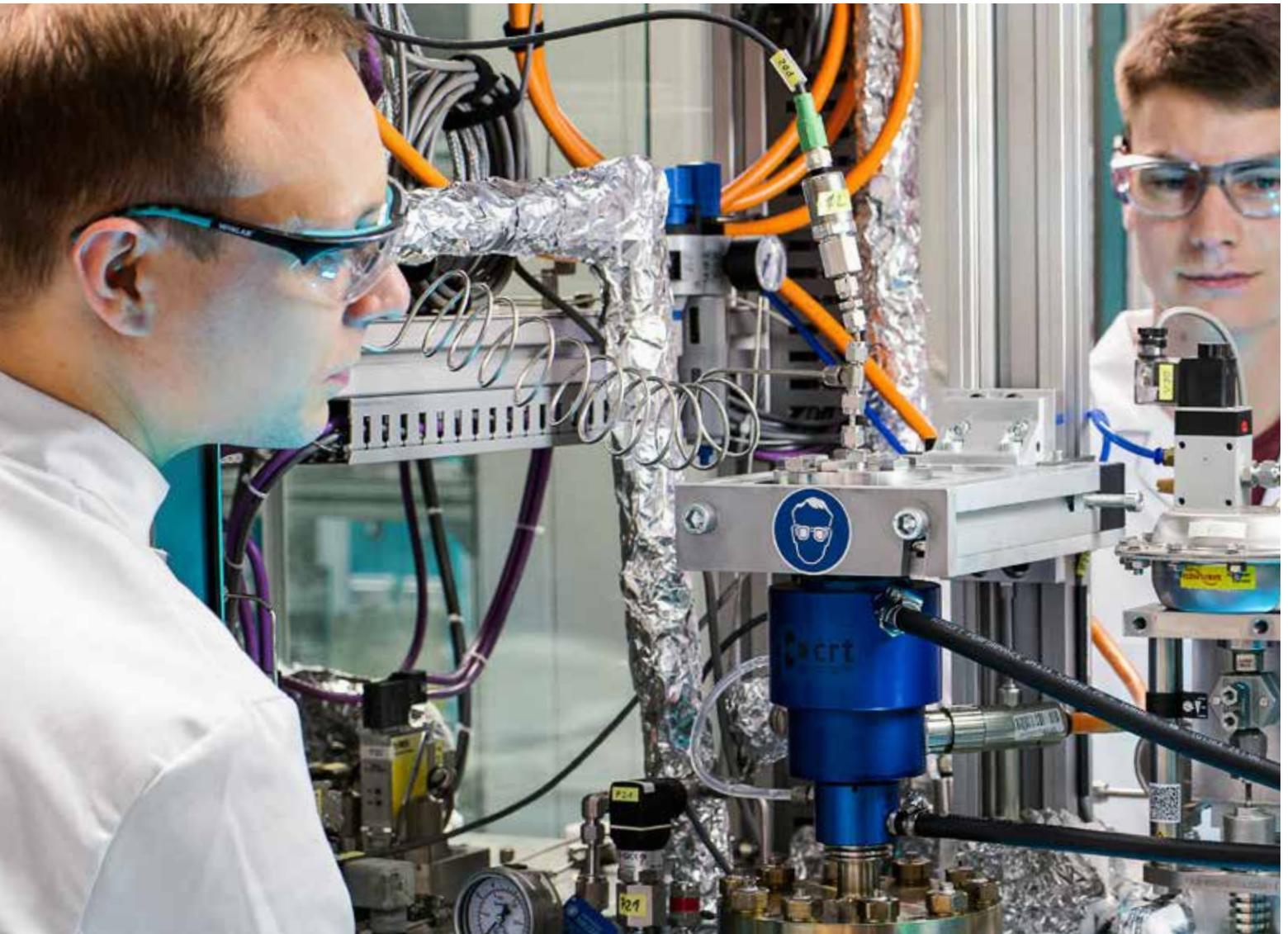




MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Report 2021 – 2022



+Lothar Kaps (left) and Wieland Kortuz (right)

Ph. D. candidates in the Physical and Chemical Foundations of Process Engineering group

Process Engineers Lothar Kaps (left) and Wieland Kortuz (right) of the Physical and Chemical Foundations of Process Engineering research group inspecting the equipment of the methanol synthesis plant prior to dynamic operation. Please read more about their research on pages 38-39 in this report.

Report 2021 – 2022

MAX PLANCK INSTITUTE
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MAGDEBURG

FREQUENTLY USED ABBREVIATIONS

Research Groups headed by MPI Directors

BPE	Bioprocess Engineering
CSC	Computational Methods in Systems and Control Theory
PCF	Physical and Chemical Foundations of Process Engineering
PSE	Process Systems Engineering

Research Groups headed by External Scientific Members

PSD	Process Synthesis and Dynamics
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Research Groups headed by Senior Scientists

ARB	Analysis and Redesign of Biological Networks
DMP	Data-driven Modeling of Complex Physical Systems
EEC	Electrochemical Energy Conversion
MSD	Molecular Simulations and Design

Max Planck Fellow Group

DRI	Data-Driven System Reduction and Identification
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Others

ATP	Adenosine triphosphate, organic compound that provides energy to drive many processes in living cells
BMBF	German Federal Ministry of Education and Research
BMWK	German Federal Ministry for Economic Affairs and Energy
CDS	Center for Dynamic Systems: Biosystems Engineering (Magdeburg)
CORE	European project: Continuous Resolution and Deracemization of Chiral Compounds by Crystallization
COST	European Cooperation in Science and Technology
CPTS	Chemistry, Physics and Technology Section of MPG
DAAD	German Academic Exchange Service
DARPA	Defense Advanced Research Projects Agency (United States)
DECHEMA	Expert Network for Chemical Engineering and Biotechnology in Germany (Gesellschaft für Chemische Technik und Biotechnologie e.V.)
ERC	European Research Council
ERDF	European Regional Development Fund (Europäischer Fonds für regionale Entwicklung (EFRE))

EXIST	University-Based Business Start-Ups (support programme of the BMWK)
DFG	German Science Foundation (Deutsche Forschungsgemeinschaft)
FVST	Faculty of Process and Systems Engineering at OVGU Magdeburg
GAMM	International Association of Applied Mathematics and Mechanics (Gesellschaft für Angewandte Mathematik und Mechanik)
IMPRS	International Max Planck Research School
LSA	German Federal State of Saxony-Anhalt
MLU	Martin Luther University Halle-Wittenberg
MPG	Max Planck Society (Max-Planck-Gesellschaft)
MPI	Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg
Omics	Various disciplines in biology whose names end in the suffix -omics, such as genomics, proteomics, metabolomics and glycomics
OVGU	Otto von Guericke University Magdeburg
SAB	Scientific Advisory Board
SFB CRC/TRR	DFG-funded Transregional Collaborative Research Center (Sonderforschungsbereich)
SIAM	Society for Industrial and Applied Mathematics
TH	University of Applied Sciences (Technische Hochschule)
TU	Technical University (Technische Universität Berlin, Technische Universität Dortmund)
UNRAVEL	European project: A Unique Refinery Approach to Valorise European Lignocellulosis



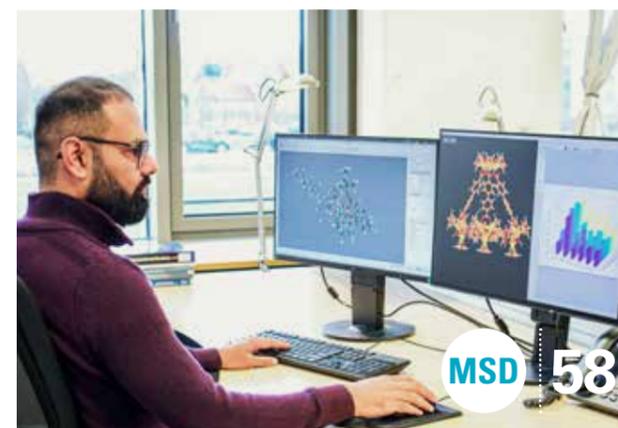
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World-class research to address societal needs in changing times

More than ever, society needs its scientists and engineers to shed light on the pressing challenges it faces, providing understanding of their causes and impacts. It also needs them to invent holistic and sustainable solutions to address these complex challenges, taking a systemic approach that accounts for all stakeholders and avoids unintended consequences. These needs have been placed in sharp focus through the COVID-19 pandemic, which has required a rapid and multi-faceted response. The acceleration of the impacts of the climate crisis are also bringing a new urgency to this mission.

The Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg is uniquely placed to respond to these challenges. The research programme has a strong core of systems thinking and systems engineering, without which it would not be possible to engineer holistic solutions. The breadth of expertise provides numerous opportunities to bring different perspectives and deep domain knowledge to bear on grand challenges. The Institute's outstanding experimental facilities offer a fast track to the testing of new ideas and their iterative improvement.

These elements must be complemented by effective leadership and a culture that encourages collaboration, communication and supports all members in contributing their ideas and energy to common goals. This latest report provides ample evidence of the Institute's ability to rise to the challenge in the midst of severe disruption, with MPI members continuing to reach beyond the Institute and to actively lead or engage in ambitious collaborative national and international projects. The Institute displayed agility in redirecting some focus to the SARS-2-COVID pandemic, deploying viral platforms for vaccine manufacturing or control strategies for contact minimization in the COVID-19 pandemic. In parallel, the Institute has continued its evolution towards enabling a more sustainable economy. Exciting progress is being made on novel manufacturing processes based on renewable resources and in the growing area of electrochemical conversion processes.

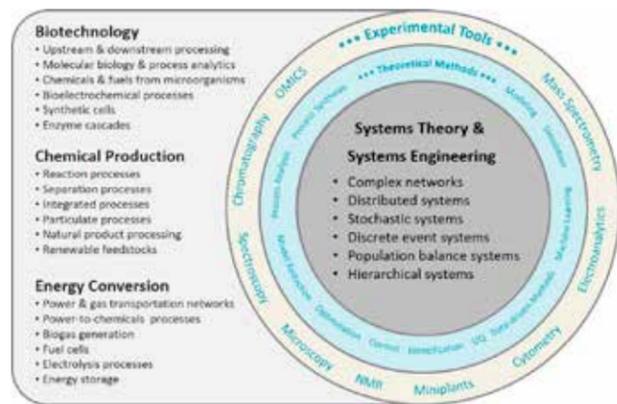
The MPI for Dynamics of Complex Technical Systems Magdeburg offers an exceptional environment in which talented researchers can make fundamental advances in our understanding of complex systems and deploy these across an impressive array of applications. This report is a celebration of the recent achievements of MPI researchers and of their commitment to shaping a better future through scientific innovation. I hope you enjoy reading it as much as I have.

Claire Adjiman

Professor of Chemical Engineering,
Director of the Sargent Centre for Process Systems Engineering
Imperial College London

+ Introduction

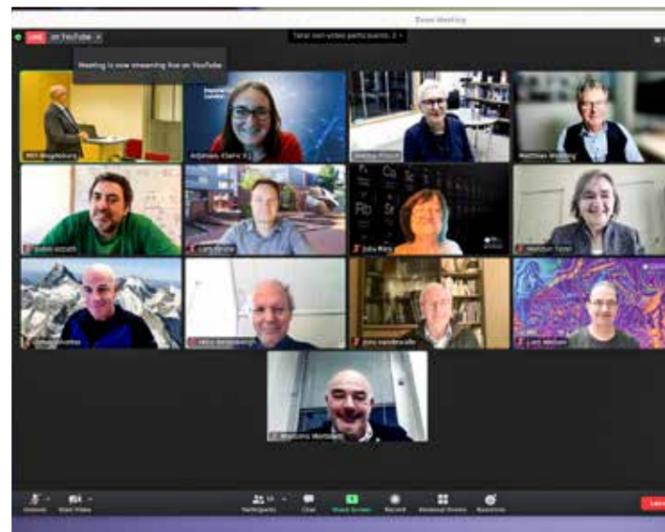
A decorative graphic consisting of several white, wavy, overlapping lines that originate from a single point on the left and spread out towards the right, set against a solid blue background.



+ **Figure 1:**
Research Concept of our institute



+ **Figure 2:**
We also report on digital event formats such as the Science Night in Magdeburg and the virtual Annual Meeting of the Max Planck Society under "Events" on pages 14 - 18.



+ **Figure 3:**
The 7th Meeting of the Scientific Advisory Board at the Max Planck Institute Magdeburg was held in November 2021 in a digital format. Shown here a screenshot of the session of the report given by the Managing Director, Prof. Peter Benner.



+ **Figure 4:**
Meeting of the Board of Trustees of our institute in May 2022: from left to right: Prof. Andreas Schuppert, Dr. Lutz Trümper, Dr. Eva E. Wille, Prof. Kurt Wagemann, Dr. Andreas Neubert, from left to right upper row: Prof. Jens Strackeljan, Dr. Michael Lehmann, Dr. Wilhelm Otten.

The Max Planck Institute in Magdeburg – Our Mission and Recent Developments

+ The global challenges arising from the increasing world population, the depletion of natural resources, and the climate change make improvements in public health and a stable supply of inexpensive pharmaceuticals, the development of sustainable production technologies, and the establishment of methods for reducing greenhouse gas emissions indispensable. The development of advanced smart processes, which allow a much more efficient and sustainable production of chemicals, transportation fuels, food and pharmaceuticals, as well as the transformation and storage of renewable energies is a formidable task for this and the next generations. Achieving breakthroughs in providing solutions to these issues requires tremendous joint international efforts comprising several scientific disciplines.

In this broad context, the main research activities carried out at the Max Planck Institute (MPI) for Dynamics of Complex Technical Systems in Magdeburg involve the development of mathematical models capable of describing complex chemical, biotechnological and energy-related processes and the analysis of the properties of these systems as well as their dynamic behavior. After validation, these models are applied to design and control efficient and sustainable production processes. Our research focus is on the following areas: chemical process engineering, bioprocess engineering, energy systems engineering, process systems engineering, systems and synthetic biology, systems theory

and control engineering, as well as scientific computing including (scientific) machine learning. The objectives of the MPI hereby do not only require the development, application and experimental validation of process and systems engineering approaches, but also the establishment of new computational methods and advances in systems and control theory, where data-enhanced methods play an increasing role. The latter has become a prominently emerging field in all areas of the Sciences and Engineering, and in the period 2021-22, we have intensified both, the development of new machine learning methods for dynamical systems as well as the use of artificial intelligence approaches in process systems engineering.

The core research concept of the MPI is illustrated in Fig. 1. Each research group of the MPI employs theoretical or/and experimental methods to analyze different complex systems involved in technical processes. Most of the studied processes belong to at least one of the system categories indicated in the center of this figure. In order to study these systems and corresponding problems, the MPI applies and develops a wide spectrum of advanced theoretical methods, represented by the inner ring.

A characteristic feature of the MPI is the direct application of theoretical methods to enable the quantitative description and model-based optimization of challenging biotechno-

logical, chemical and energy-related processes. Moreover, there is an arsenal of experimental tools applied (outer ring of Fig. 1) to validate the derived theoretical models and to quantitatively describe the processes investigated. Several of these tools are totally new, and thus are themselves subject of our research activities. We believe that the systems-oriented approach, which serves as an umbrella for all activities in the different research groups, as well as the tight integration of theoretical and experimental investigations are key factors for the success of our MPI.

Research groups

As of December 2022, the MPI consists of ten research groups: four groups headed by MPI Directors (Profs. Benner, Reichl, Seidel-Morgenstern, Sundmacher), three groups headed by Senior Scientists (Dr. Klamt, Prof. Stein, Dr. Vidaković-Koch), a newly established Max Planck Research Group (MPRG) headed by Dr. Nüske (see below), one group headed by an External Scientific Member (Professor Kienle) and, until December 31, 2022, one group headed by a Max Planck Fellow (Professor Antoulas).

In August 2022, the MPRG "Data-driven Modeling of Complex Physical Systems" (DMP) was established at the Institute under the leadership of Dr. Felix Nüske. The group is concerned with computational methods for the analysis

and simulation of complex systems at the atomic or molecular level. In particular, the fundamental challenges posed by high-dimensional state spaces, large time-scale differences, and considerable model uncertainties are to be addressed with the help of new mathematical approaches and machine learning methods, thus strengthening the MPI activities in the direction of data-enhanced and data-driven sciences.

SARS-CoV-2 Pandemic

Of course, the pandemic had a major impact on the operation of our Institute. Nevertheless, we never had to close the MPI due to careful protection measures and distance rules, working in shifts, and using flexible mobile working options. Also, the use of digital formats for meetings and seminars as well as social events was quickly adopted with the help of our IT department. Of course, during this time many events were held virtually like the Science Night 2021 (see Fig. 2), the meeting of our Scientific Advisory Board (see Fig. 3 and the report below), as well as one meeting of our Board of Trustees (see Fig. 4-5 and the report below). The number of experiments had to be reduced, but experimental work could continue all the way through. In 2022, we could re-start many on-site meetings by following the given restrictions due to the pandemic. This included the "Zukunftstag – Girls' und Boys' Day" 2022 (Fig. 6) and the Science Night 2022 (Fig. 7), which will be described in more



+ Figure 5: During the meeting of the Board of Trustees on 5 May 2022, Prof. Peter Benner expressed his thanks to Dr. Lutz Trümper, at that time still Lord Mayor of the state capital Magdeburg, for his committed participation in the Board of Trustees of the Institute.



+ Figure 6: Ten pupils from 7th to 10th grades from Magdeburg, Burg and Dessau took part in our offer for the nationwide Future Day (Zukunftstag – Girls' und Boys' Day) on 28 April 2022 - in compliance with Corona safeguards. The students as well as the organizers at the MPI were all the more pleased to once again gain an insight into the natural sciences and engineering research fields as well as the technical fields of work on site and with close personal contact.



+ Figure 7: Our institute opened the doors to the people of Magdeburg as part of the 16th Science Night on 11 June 2022. On site, visitors could simulate and model the COVID pandemic and the SARS-CoV-2 virus themselves or learned about methods for environmentally friendly manufacturing processes and circular economy.



+ Figure 8: Members of staff in the main hall of our institute in November 2022.

detail on pages 14-18 in the section "Events". Meanwhile, we could return to normal operation with regular in-person working conditions at the Institute (see Fig. 8), while keeping flexible options for mobile working where possible!

We also started several research projects with the goal of mitigating certain effects of the pandemic. To name two examples, in the EXIST Project ContiVir, the BPE department investigated "Enabling Bedside Manufacturing of Viral Vaccines & Gene Therapies", while the CSC department contributed to the BMBF B-FAST project "Risk-based Surveillance of Population Groups" that investigated optimal testing strategies for the personnel in a locked ward, using the example of the Magdeburg child and adolescent psychiatry clinic.

Visit of the Scientific Advisory Board 2021

The seventh visit of the Scientific Advisory (SAB) of the MPI took place November 22-24, 2021, as part of the evaluation of the Research Field VI of the Max Planck Society's Chemical-Physical-Technical Section. As the SARS CoV-2 pandemic was still fully going on, it was decided early in 2021 to hold the SAB meeting online via zoom sessions and breakout rooms. Given that the locations of SAB members ranged from Brisbane in Australia to San Jose in California, USA, thus covering 18 time zones, this caused a major organizational effort. Fortunately, the flexibility of our SAB members allowed to cope with this, using

individual sessions with the research groups and by only meeting for a few plenary sessions, see Fig. 3. Despite all difficulties, the virtual SAB meeting and site visit happened in a constructive and supportive atmosphere. The outcome for the MPI was that the SAB rated the Institute's research results and agenda as "outstanding" - the best rating achievable. Quoting from the SAB report, the SAB

- + "commends the high quality work that is produced [...] it finds the research outputs to be outstanding. The combination of world-leading computational work with excellent experimental facilities is a unique strength of the Institute that differentiates it from other centres of excellence in this research field"
- + "is highly supportive of the future research directions identified by the MPI team. Specifically, high performance computations and data science have an important role to play ..."
- + "commends the Institute for the very high level of expertise of its personnel."

We gladly accept these commendations as a recognition for the research we have done, but more than that as an incentive to maintain our scientific level and to further develop our research efforts. These will then be presented at the next SAB visit in November 2024, then hopefully in-person and on-site!

Board of Trustees

The Institute's Board of Trustees advises the Institute in social and political aspects. The board consists of high ranking representatives of the state government, the science community, industry, and media. After an online meeting in December 2020, we postponed its next meeting until May 2022 in the hope to be able to meet in-person. We were more than glad that this became indeed possible, see Fig. 4. In particular, as the long-term chair of the Board, Dr. Lutz Trümper, Lord Mayor of the City of Magdeburg retired at the end of June 2022, we had the possibility to thank him for all his support of the Institute in person, and could hand over some farewell gifts, see Fig. 5. All in all, discussions with the Board of Trustees have always been fruitful and constructive, and we thank all members of the Board, now chaired by Prof. Kurt Wagemann (DECHEMA) for their continued efforts to further develop the Institute's agenda and its research visibility.

In conclusion, the years 2021-22 were challenging in multiple ways, with the SARS-CoV-2 pandemic as reported above and the Russian war of aggression on Ukraine affecting the Institute's operation in several ways. As for the war in Ukraine, we tied our relations to its National Academy of Sciences (NAS) and are hosting several Ukrainian scientists after fleeing from Sloviansk, the pre-war location of the NAS Institute for Applied Mathematics and Mechanics. Despite all crises, our successful research activities continued,

and led to numerous high-level results, some of which are discussed in more detail later in this report. For the coming years 2023-24, I wish my successor in the position as Managing Director, Kai Sundmacher, all the best and hopefully a smoother operation without further crisis on a global scale! Moreover, we all look forward to celebrating the 25th anniversary of the institute in 2023! If you want to learn more about the history and 25 years of operation of the MPI in Magdeburg, I highly recommend the special section at the end of this report, with many of the highlights since 1998!

Peter Benner

Magdeburg, Juni 2023

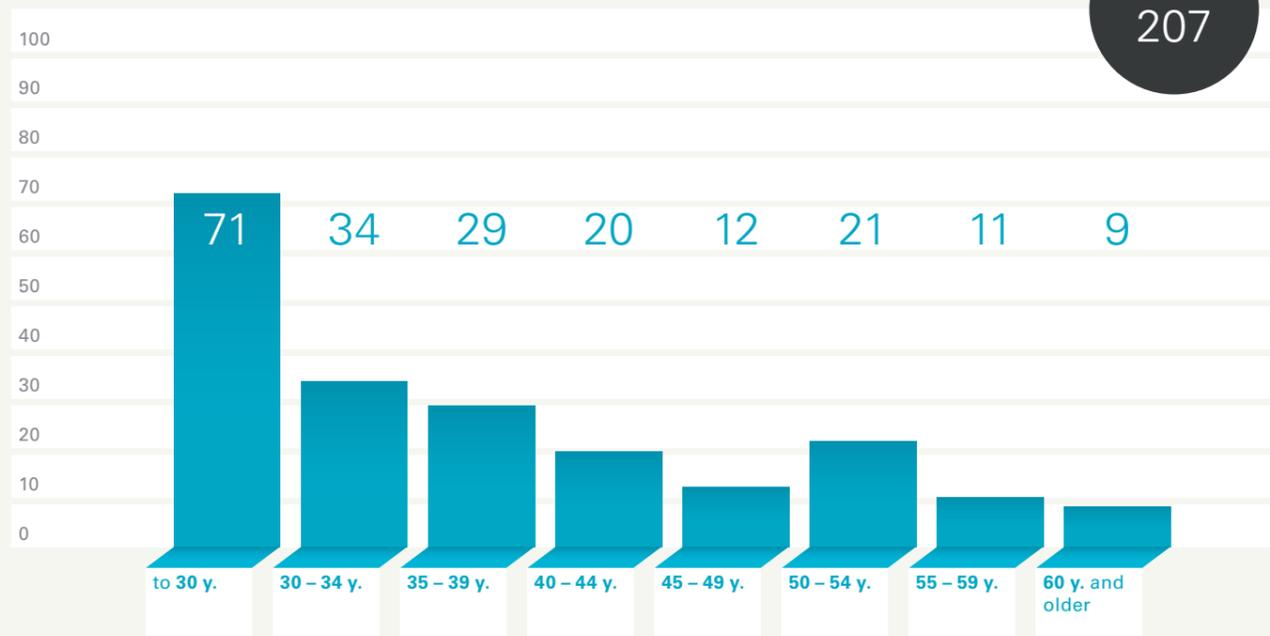
Prof. Dr. Peter Benner
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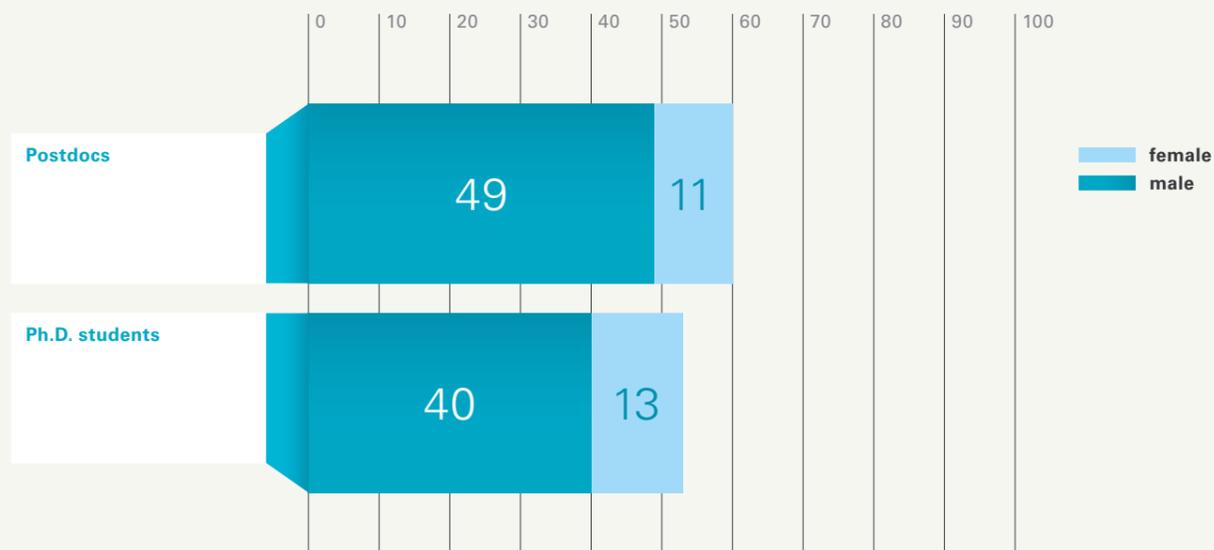


+ Facts and Figures

STAFF
Age structure of the workforce at the MPI (as of December 31, 2022)



STAFF
Distribution of scientists by gender
Female employees: 18% Postdocs and 25% Ph.D. students

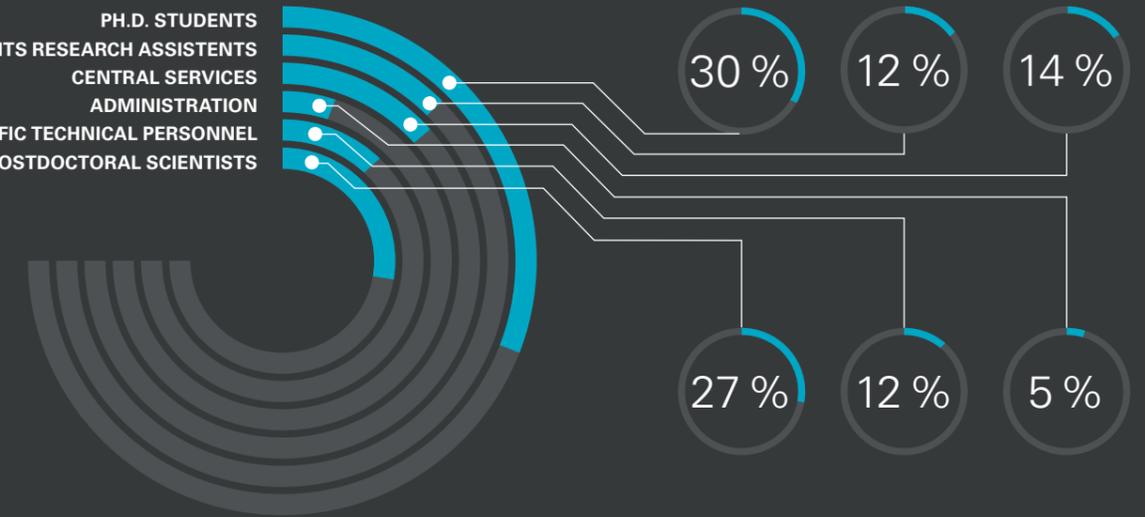


The two graphs above show the age structure and the gender balance among the institute's scientists on the Postdoc and Ph.D. levels, respectively. As Max Planck Institutes are run with very few permanent scientists, the average age of employees is quite low as the majority of scientists consists of Ph.D. students and young Postdocs.

STAFF
December 31, 2022: 207 Employees

- PH.D. STUDENTS
- STUDENTS RESEARCH ASSISTANTS
- CENTRAL SERVICES
- ADMINISTRATION
- SCIENTIFIC TECHNICAL PERSONNEL
- SENIOR/POSTDOCTORAL SCIENTISTS

113 Scientists: 60 Postdocs, 53 Ph.D. students



At the end of 2022, the MPI employed 207 persons. The majority are scientists and student researchers as illustrated by the pie chart above. As can be seen, the institute is run by a lean administration, while operating the labs and technical facilities accounts for the rest of the employees.

EXPENDITURE PATTERN IN 2022
Total Expenses in Fiscal Year 2022: 15.95 million Euro



The total budget of the MPI in the fiscal year 2022 was 15.95 million Euro. The pie chart above shows how this was distributed to the major budget categories. As can be seen, more than 70 % of the budget was used for salaries.

MPI-GENERAL BUDGET 2022
Total Revenue: 15.95 million Euro
Third-party funds: 2.7 million Euro



This pie chart related to the budget shows the distribution of the budget sources. As usual for Max Planck Institutes, the main source is institutional funding provided by the Max Planck Society.

+ Selected Events 2021 – 2022

New Digital Formats in 2021: Science Night and Opening Lectures Streamed Live

The Science Night in Magdeburg, initiated in 2006 by the City of Magdeburg and the scientific institutions, is an integral part of our science communication activities. In 2019, we attracted 1,319 visitors to our institute.

The COVID-19 pandemic in 2020 and 2021 had severe impact on our outreach activities. In accordance with German health precautions and the recommendations of the Max Planck Society, we had to cancel or postpone all events from the middle of March 2020 onwards. The 15th Science Night in Magdeburg, originally scheduled for June 6, 2020, was canceled too.

To offer a new format independent of the pandemic, the City of Magdeburg and the scientific institutions planned a virtual platform with a mixed program of livestreams, panel discussions, interactive experiments, and podcasts. On May 29, 2021, the 15th edition of Science Night in Magdeburg streamed a total of 18 hours of live events on three channels, broadcasted from three studios. More than 60 exciting program items revolved around current scientific developments, latest research projects, and social debates. We contributed videos, demos, home stories, interviews, lectures, and live talks explaining the state-of-the-art of our research. More than half a year of conception, planning, and creation finally paid off: in total, 6,000 devices/spectators from Magdeburg and around the globe clicked onto the livestream.

On June 23, 2021, our labs turned into a broadcasting studio. Members and committees of the Max Planck Society had to



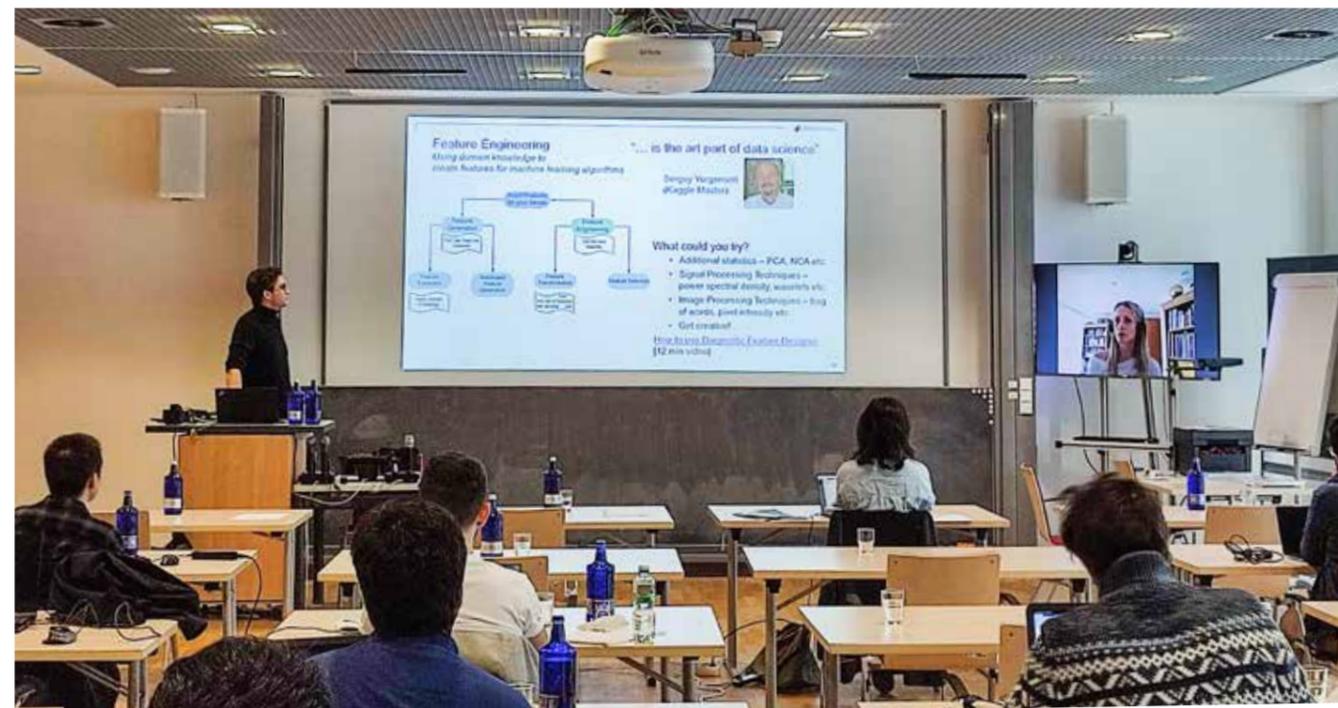
+ Prof. Udo Reichl was connected live into the studio to Prof. Martin Stratmann, President of the Max Planck Society, and Prof. Klaus Blaum, Vice President of the Max Planck Society, on 23 June 2021.

meet digitally for their 72nd Annual Meeting, so the opening lecture on the topic “Cell Culture-based Virus Production Revisited: Applications, Needs, Chances and Challenges”, given by Prof. Dr.-Ing. Udo Reichl, was streamed live. The Annual Meeting with 600 participants was originally intended to take place on-site in Magdeburg, with meetings in the MARITIM Hotel Magdeburg and with guided tours through our institute. Unfortunately, all local arrangements and activities had to be canceled due to the pandemic. The 76th Annual Meeting is scheduled for 2025 to take place in Magdeburg.

| Gabriele Ebel

IMPRS Summer School 2021 on Machine Learning for Process and Systems Engineering

The biannual IMPRS Summer School took place in a hybrid format on September 27–29, 2021. Researchers from the International Max Planck Research School for Advanced



+ The IMPRS Summer School on Machine Learning for Process and Systems Engineering was held in a hybrid format on September 27–29, 2021 at our institute.

Methods in Process and Systems Engineering participated in person and non-IMPRS members were able to follow all the lectures online via a live stream.

In 11 different lectures and tutorials, outstanding experts shared their knowledge and competencies relating to the overall topic of Machine Learning for Process and Systems Engineering. Ph.D. student Metehan Ilter said: “The IMPRS Summer School broadened my perspective on the math behind machine learning and on its wide application areas across different engineering disciplines”.

The Summer School started with a welcome address by Prof. Dr.-Ing. Kai Sundmacher, the spokesperson of the IMPRS. Five outstanding lectures - ranging from the basic principles of machine learning and an introduction to computational intelligence methodologies through to special requirements for Gaussian processes and physics-informed learning - made this day a valuable experience.

On the second day, interesting tutorials on the introduction to artificial intelligence in MATLAB and how to use it were given. A fascinating lecture on Data-Driven Optimization in Dynamic Systems: Solutions, Structure, and Control, given by Julius Martensen and Sebastian Sager of Otto von Guericke University Magdeburg, rounded off the day.

The IMPRS members then gathered for a social event. A scientific scavenger hunt introduced some of the most interesting scientists with connections to Magdeburg throughout the city’s history. All participants reported that they had a lot of fun solving the different tasks for clues to the next destination.

On the third day, three different lectures on machine learning approaches, given by scientists and members of the OVGU, RWTH Aachen, and Swiss company *datahow*, rounded off the IMPRS Summer School perfectly. | Michelle Bäumer

SmartProSys Symposium 2022: Towards Sustainable & Circular Production Processes

On March 2–4, 2022, the SmartProSys research initiative hosted the symposium “Smart Process Systems Engineering: Towards Sustainable & Circular Production Processes”. Due to the ongoing COVID-19 pandemic, an online format was chosen. All the conference sessions were held in the afternoon so that colleagues in the Western Hemisphere were able to participate.

The event was opened by a representative of the Saxony-Anhalt Ministry of Science, Energy, Climate Protection and the Environment. The program consisted of six thematic sessions: Mechanical & Thermal Preprocessing, Chemical & Biological Decomposition Processes, Chemical & Biological (Re-)Synthesis, Systems Engineering & Computational Methods, Supply Chain & Sustainability Management, and Circular Society.

In each session, two guest speakers and two SmartProSys speakers presented the latest state of their research. The guest speakers came from renowned scientific institutions in Germany and abroad, including RWTH Aachen University, the University of Cambridge, University College London, Imperial College London, Cornell University (New York) and the Norwegian University of Science and Technology (Trondheim). A special highlight was the presentation by Prof. Dr. Peter Seeberger from the MPI of Colloids and Interfaces in Potsdam.



+ Kick-off and first in-person meeting of ProteoCure, the new EU COST (European Cooperation in Science and Technology) Action in Ljubljana, Slovenia, from 17-19 May 2022



+ GAMM Workshop on Computational and Mathematical Methods in Data Science (COMinDS) on November 3rd and 4th, 2022 at the Max Planck Institute in Magdeburg.



+ The participants of the 2nd International Symposium on „Insights into Gas Diffusion Electrodes“ in front of the Johanniskirche in Magdeburg on 6 September 2022.

The usual format of a poster session at an in-person conference was replaced by flash presentations. In the two sessions “Technology & Engineering” and “Management & Social Sciences”, young scientists had the opportunity to present their own research work. The keynote lectures and short presentations were complemented by a panel discussion entitled “Challenges of the chemical industry on the way to a circular economy” which dealt with the applications of a circular economy in the chemical industry. Experts from industry and policy advisors were invited. A total of 133 participants registered for the event. However, attendance varied across different sessions, with the highest number of concurrent participants being 85.

! Dr. Jakob Schweizer

<https://www.smartprosys.ovgu.de/symposium2022program.html>

Kick-off Meeting of the ProteoCure COST Action

ProteoCure, the new EU COST (European Cooperation in Science and Technology) Action, brings together European researchers from academia, clinics and industry to develop new approaches and strategies to selectively control the proteolysis (i.e. protein degradation) for therapeutic or biotechnological purposes.

Malfunctioning of the proteolysis machinery leads to an accumulation of deleterious proteins or, in the opposite, to an excessive degradation of beneficial proteins. These regulatory proteins are implicated in multiple human diseases such as cancers, neurodegeneration, developmental and aging disorders, as well as in infectious diseases. New therapeutic approaches are required to maintain and control the proteolytic machinery.

During the kick-off and first in-person meeting in Ljubljana, Slovenia, from 17-19 May 2022, more than 100 European scientists were discussing approaches and strategies for scientific exchange and definition of common protein targets.

! Dr. Matthias Stein

2nd International Symposium on Electrodes for Electrolysis and Fuel Cells in Magdeburg

On September 5–7, 2022, researchers from the fields of materials science, electrochemistry, and process engineering met in Magdeburg for the second time since 2019 for the International Symposium on Insights into Gas Diffusion Electrodes – From Fundamentals to Industrial Applications. The event was focused on research for the energy transition and the circular economy. It was organized by Tanja Vidaković-Koch from the Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, and Thomas Turek from the Clausthal University of Technology (TU Clausthal) within the framework of the DFG Research Group 2397 “Multiscale Analysis of Complex Three-Phase Systems”.

The German Research Foundation has funded this research group since 2016. The scientists aim to gain new insights into the complex processes within gas diffusion electrodes through experiments and simulations. The focus of the work in the second phase of the project is the electrochemical conversion of CO₂ to CO as an important value-added product for the chemical industry.

In lectures, presentations, and poster contributions, 100 scientists from 11 nations as well as representatives and speakers from various industrial companies including DE NORA, Elogen, Avantium, SGL Carbon, and Johnson Matthey discussed the latest developments in the field

of gas diffusion electrodes. Three poster prizes for young scientists were awarded during the symposium at the Johanniskirche event center. ! Dr.-Ing. Tanja Vidaković-Koch and Prof. Thomas Turek

The First MaRDI Workshop on Scientific Computing

With the ever-growing body of scientific knowledge and explosion of data generated by computer-based experiments, the Findability, Accessibility, Interoperability, and Reusability (FAIR) principles of research data have become key factors for further scientific progress. In scientific computing, numerical algorithms and their implementations, as well as procedural data and their metadata descriptions, are regarded as central research data, in addition to simulation data themselves. Establishing FAIR principles for all these data is the aim of the task area “Scientific Computing” within the Mathematical Research Data Initiative (MaRDI).



+ Participants of the 1st MaRDI Workshop on Scientific Computing, 26-28 October 2022, in Münster.

The First MaRDI Workshop in Scientific Computing, hosted 26-28 October 2022 by the Mathematics Münster Cluster of Excellence in Münster, Germany, brought together 46 researchers from scientific computing and related disciplines. Participants delivered talks related to knowledge graphs and ontologies, software interfaces, benchmarks, formal workflow descriptions, software distribution, reproducibility, and research data management. In addition to presentations on current MaRDI projects and selected keynote talks, breakout sessions inspired stimulating discussions about the imminent challenges MaRDI faces.

For more information about FAIR principles and MaRDI, please visit <https://www.go-fair.org/fair-principles/> and <https://www.mardi4nfdi.de/about/mission>. ! Dr. Kathryn Lund

GAMM Workshop on Computational and Mathematical Methods in Data Science (COMinDS)

After the COVID-19 pandemic, an in-person GAMM annual workshop was organized at Max Planck Institute, Magdeburg, on November 3rd and 4th, 2022. It was the third in a series of workshops run by the GAMM activity group COMinDS. Prof. Dr. Martin Stoll and Prof. Dr. Gitta Kutyniok started the COMinDS activity group in 2019. Its two previous workshops were held in Berlin and Leipzig. The focus of the third workshop was aligned with the aim of COMinDS, i.e. to bring people from Europe together to link fundamental methodologies from different areas, ranging from applied (machine learning) to theoretical (algebraic geometry) mathematics. The efforts of many outstanding researchers are currently focused on building intelligent systems. The aspiration is to develop advanced algorithms in order to enrich theoretical AI and bridge the gap between the theoretical development of AI and its implementation in the physical world.



+ Panel discussion with the speakers (from left to right) Achim Kienle (OVGU, Magdeburg), Erich Fischer (OHplus, Staßfurt), Gerd Unkelbach (UPM, Leuna) and Henning Wilts (Wuppertal Institute), who contributed via video conference. The panel discussion was moderated by Jakob Schweizer (MPI Magdeburg).



+ Group picture of the participants who attended in presence the DEHEMA Regional Colloquium on 10 November 2022.

The scientific program included 11 talks and three invited speakers: Prof. Dr. Sebastian Trimpe from RWTH Aachen, Prof. Nicolas Gillis from the University of Mons and Prof. Dr. Andrea Beck. Unfortunately, the third speaker was not able to attend in person. The talks covered a range of interesting research topics: from Dynamical systems to Non-negative Matrix Factorization, from Gaussian Processes to Spiking Neural Networks. The various applications of the work presented and perspectives from different field experts created an engaging environment. A friendly atmosphere and scientific discussions at the workshop fostered stronger ties among institutes/researchers.

Many scientists took part in the GAMM workshop, from well-known experts in the field to new Ph.D. students from different parts of Europe. During the workshop, a hybrid business meeting was also held by Prof. Dr. Stoll. The onsite election of a new chair was conducted and Prof. Dr. Axel Klavonn from the University of Cologne humbly accepted the role. A number of responsibilities relating to the representation of GAMM at conferences such as SIAM and ILAS and the organization of future events were cordially accepted by early career GAMM members. Thirty-four out of 39 registered researchers gathered at the institute. All the above-mentioned contributions and support from the MathCoRe@OVGU DFG research training group made this workshop a successful event. | **Kirandeep Kour**

Regional Colloquium: Sustainable Production of Chemicals and Materials

On November 10, 2022, the Magdeburg research initiative SmartProSys and the Society for Chemical Engineering and Biotechnology (DECHEMA) organized a regional colloquium on “Smart Process Systems: Sustainable Production of Chemicals and Materials” at the Max Planck Institute in

Magdeburg. The participants were scientists from diverse fields within the natural, engineering, and human sciences, as well as representatives from state agencies, civil society organizations, and the economy whose main focus was the chemical industry in Central Germany.

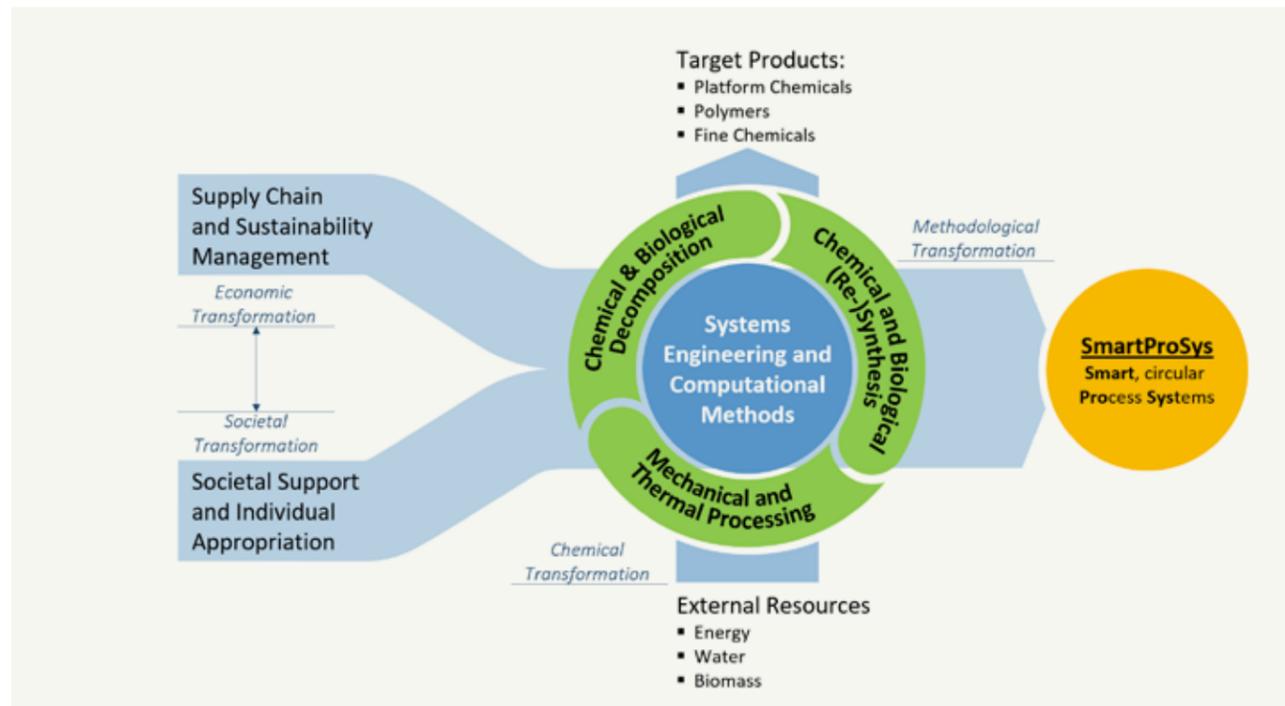
In the Research session, four speakers from the engineering sciences spoke about developments in the field of sustainable production: Prof. Dr.-Ing. Kai Sundmacher (MPI Magdeburg), Prof. Dr.-Ing. Achim Kienle (OVGU Magdeburg), Prof. Dr. Klaus Kümmerer (Leuphana University Lüneburg), and Dr.-Ing. Sylvia Schattauer (Fraunhofer Institute for Wind Energy Systems IWES, Leuna).

In the Industry session, the challenges of sustainable transformation were discussed using three examples: the production of synthetic tire rubber (Dr. Malte Wohlfahrt, Synthos Group, Schkopau), the use of renewable raw materials such as wood (Dr. Gerd Unkelbach, UPM Biochemicals GmbH, Leuna), and the synthesis of fine chemicals as valuable by-products in the processing of biofuels (Erich Fischer, OHplus Staßfurt).

In the Society & Politics session, Dr. Henning Wilts (Wuppertal Institute for Climate, Environment, Energy) gave an introduction to the political framework conditions for a circular economy in the chemical industry. The program ended with a panel discussion with the speakers on next steps towards the sustainable production of chemicals and materials. After the event, the participants had the opportunity to exchange ideas over beer and pretzels. In total, 36 people participated in person and about 100 people participated online. | **Dr. Jakob Schweizer**

https://www.smartprosys.ovgu.de/dechema_regionalkolloquium_2022.html

+ Research Groups



SMARTPROSYS: A JOINT RESEARCH INITIATIVE WITH OTTO VON GUERICKE UNIVERSITY

Since spring 2021, the Max Planck Institute is contributing to the preparation of “SmartProSys: Smart Process Systems for a Green Carbon-based Chemical Production in a Sustainable Society”, a joint research initiative with the Otto von Guericke University and several other research institutions. This project aims at exploring and developing new production systems for a climate-friendly chemical industry. The key idea of SmartProSys is to defossilize today's chemical production by transforming it into a multi-circular system that, in its final stage, must be fed exclusively by renewable carbon resources and renewable energy.

The chemical industry is facing major challenges and massive structural change. The environmentally and climate-friendly manufacture of chemical products has long been an issue for society, politics and business. In addition, there are other challenges: The current war in Ukraine and the energy crisis are hitting the chemical industry with full force, but are bringing to light a problem that has been apparent for a long time, namely that of security of supply for the chemical industry with raw materials and energy carriers.

The central strategy of SmartProSys is the transformation of energy-intensive, linear process chains based on fossil raw materials and energy sources to sustainable, fully closed, energy-saving cycles of all molecular building blocks using biomass, residual materials and renewable energies. To achieve this, we need not only innovations in the fields of

chemistry, process engineering and control engineering, but also the know-how of computer science, mathematics, logistics and business management. Since this transformation can only succeed with people and society as a whole, the expertise of political science, sociology and psychology is also necessary. For this reason, scientists from a wide range of disciplines have joined forces in Magdeburg to develop new concepts and methods for a climate-friendly chemical industry.

SmartProSys aims to explore the scientific basis for the successful establishment of smart process systems for sustainable chemical production in the context of the circular economy and to develop new methods for the design, analysis and operation of these systems and to demonstrate their effectiveness for various process examples for the conversion of renewable raw materials (biomass, residues, waste streams) into selected target products (bulk chemicals, fine chemicals, polymers). This framework requires the holistic system-oriented consideration of closed-loop systems, taking into account all essential technological, economic, sociological and sustainability-relevant aspects.

In SmartProSys, the Max Planck Institute for Dynamics of Complex Technical Systems (MPI-DKTS) collaborates with the Otto von Guericke University, the Leibniz Institute of Catalysis (LIKAT, Rostock), the Fraunhofer Institute for Factory Operation and Automation (IFF, Magdeburg), the Helmholtz Centre for Environmental Research (UFZ, Magdeburg/Leipzig) and several individual researchers from other institutions. A total of about 50 university professors and

+ Figure 1:

The research concept of SmartProSys is focused on the circular processing of components and materials essential for the future “net zero” chemical industry, in particular carbon and its compounds. Three main processing stages are necessary to keep materials in circulation: (i) mechanical and thermal preprocessing of waste and renewable stock feeds such as biomass, (ii) chemical-biological decomposition to building blocks, and (iii) chemical-biological (re-)synthesis of new products. Advanced systems engineering and computational methods, including artificial intelligence and machine learning, will be used for designing, operating and optimizing the conversion processes along the processing cycle. Furthermore, next-generation supply systems will be developed and the sustainability of new production processes will be assessed. Finally, the transformation to a “net zero” chemical industry is only possible if the societal support and individual appropriation of recycling is ensured.

Authors

Prof. Dr.-Ing. Kai Sundmacher

Kai Sundmacher studied mechanical and process engineering at the University of Hannover and the TU Clausthal. After his doctorate, he served as scientific head of the research groups “Reactive Distillation” and “Electrochemical Engineering” at the Institute of Chemical Process Engineering at the TU Clausthal. In 1999, he was appointed to the professorship of Process Systems Engineering at Otto von Guericke University Magdeburg and since 2001, Kai Sundmacher has been Director at the Max Planck Institute in Magdeburg and Scientific Member of the Max Planck Society. Since 2021, Kai Sundmacher acts as spokesperson of SmartProSys.

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Prof. Dr.-Ing. Achim Kienle

Achim Kienle studied process engineering at the University of Stuttgart. After his doctorate, he became head of the “Process Synthesis and Process Dynamics” group at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg. In 2002, he was appointed to the professorship for automation technology/modeling at Otto von Guericke University in Magdeburg, followed by his appointment as an External Scientific Member of the Max Planck Institute in Magdeburg in 2007. Since 2021, Achim Kienle acts as spokesperson of SmartProSys.

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Dr. Jakob Schweizer

Jakob Schweizer studied physics with a focus on biophysics at the TU Dresden, the University of Leipzig and the Université Denis Diderot in Paris. After his Ph.D. in synthetic biology, he conducted research in cell biology at Oxford University. From 2014 to 2021, he served as scientific coordinator of the Max Planck Research Network for Synthetic Biology (MaxSynBio). He then took over the scientific coordination of the SmartProSys research initiative. Since 2023, Jakob Schweizer has been research coordinator at the Max Planck Institute in Magdeburg.

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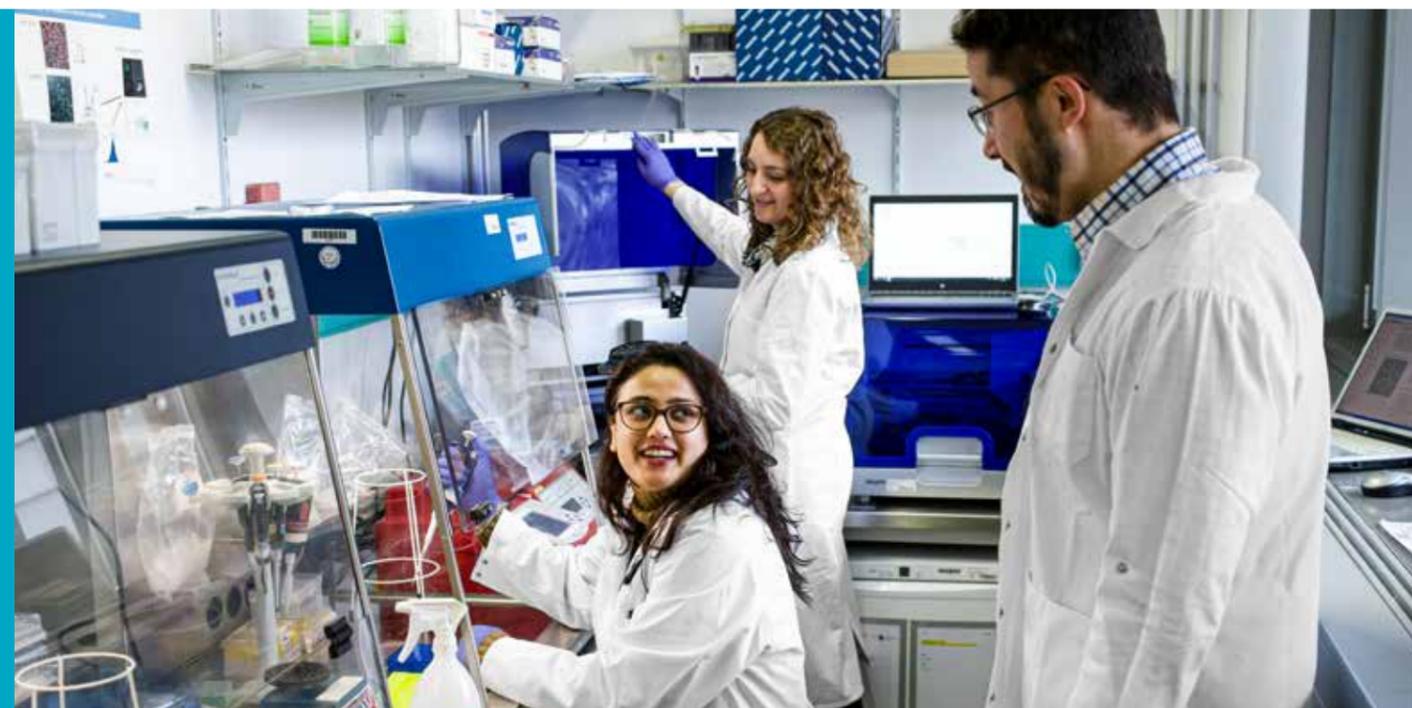
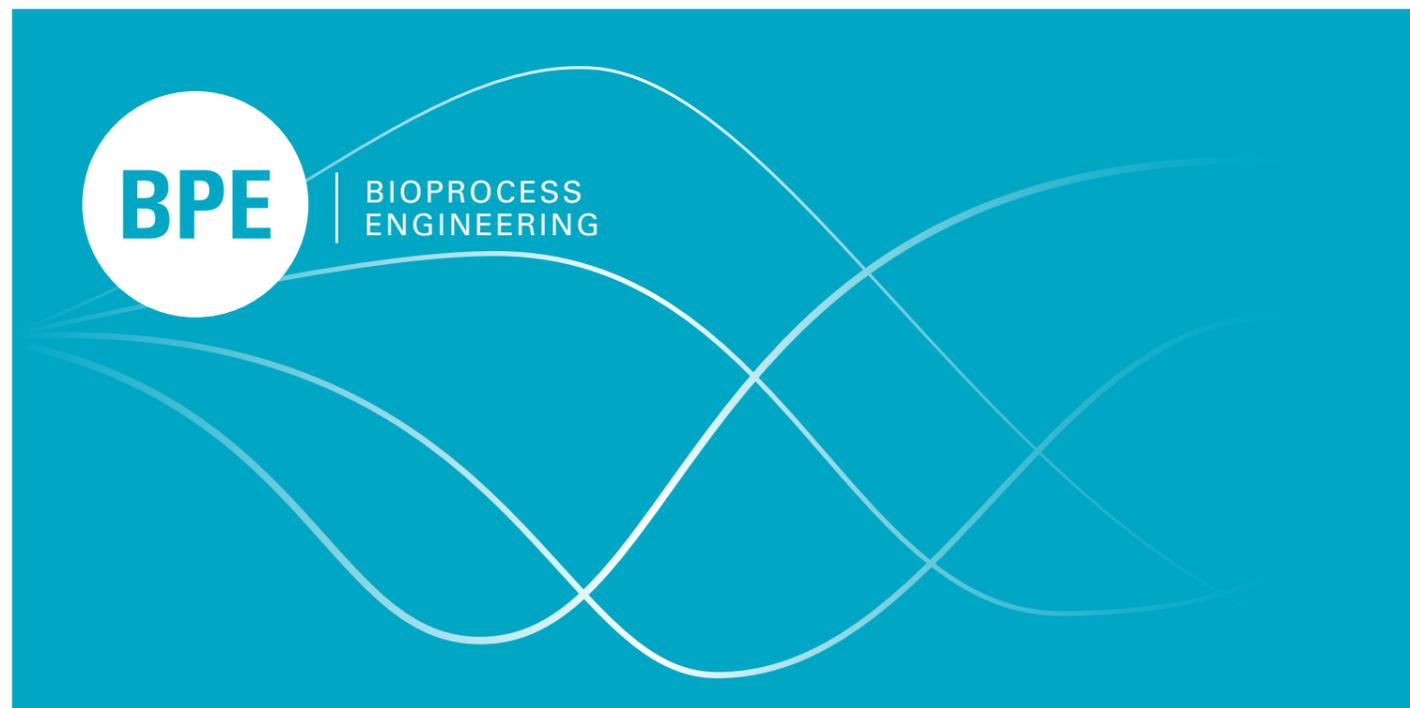
group leaders from the participating institutions contribute to the development of the SmartProSys research initiative. Furthermore, we strive for a cooperation with the new “Center for the Transformation of Chemistry (CTC)”, which will be established in Delitzsch under the direction of Prof. Peter Seeberger (MPI of Colloids & Interfaces).

The scientists participating in SmartProSys attach great importance to the exchange among each other, but also with external colleagues. Since November 2021, regular research colloquia have been held in which the participating scientists present their ideas. Staff and students of all participating scientific institutions in Magdeburg have been invited to attend the colloquia. Moreover, a first international symposium was organized from March 2-4, 2022, in a virtual format due to the Covid 19 pandemic (see “SmartProSys Symposium”). A second symposium - likely in physical format - is scheduled for December 2023. On November 10, the research initiative, in cooperation with DECHEMA/Frankfurt am Main, hosted a regional colloquium at the Max Planck Institute that focused on the challenges that the chemical industry in the region is facing, and how to implement the transformation. Guests from industry, politics and civil society in particular were invited to this event (see “DECHEMA Regional Colloquium”).

Although the challenges outlined above affect the chemical industry to the same extent all over the world, they are particularly relevant for Germany. After all, here the chemical industry represents an indispensable pillar of the economic system - in the past as well as in the present. This is particu-

larly true for the region in the immediate vicinity of Magdeburg's Max Planck Institute: Central Germany is one of the most important locations for the chemical industry. Thus, the state of Saxony-Anhalt therefore has an original interest in a future-oriented “Net Zero” transformation of the chemical industry in Central Germany. For this reason, the Ministry of Science, Energy, Climate Protection and the Environment of Saxony-Anhalt is supporting the SmartProSys initiative with start-up funding, with the help of which it has already been possible to launch initial bridge projects between the participating scientists from different disciplines. The MPI would like to take this opportunity to express its sincere thanks for the great support of the state!

More information on the SmartProSys research initiative: <https://www.smartprosys.ovgu.de> | Prof. Dr.-Ing. Kai Sundmacher, Prof. Dr.-Ing. Achim Kienle, Dr. Jakob Schweizer



+ Molecular biologist Tanya Dogra designs and generates genetically engineered vector-based antivirals, which can be produced in cell culture-based production processes. The research activities of the Molecular Biology team are introduced on the following pages.

PROF. DR.-ING. UDO REICHL | DIRECTOR

Bioprocess engineering covers the use of microorganisms in the manufacturing of industrial bulk products, food and biopharmaceuticals. In addition, bioprocess technology plays an important role in biogas and biofuels production, wastewater processing and solid waste treatment. The design and optimization of bioprocesses from both an engineering and a biological point of view requires an integrated view of complex biological systems, in-depth understanding of (bio)chemical reactions, dedicated equipment and modeling tools. Additionally, a wide range of assays for process monitoring and a comprehensive set of analytical and “omics” technologies should be utilized. The challenges we are facing today in bioprocess engineering relate not only to the increase in product yields, but also to the establishment of new methods for process intensification and a reduced time to market while guaranteeing the quality and safety of drugs.

In the context of biopharmaceuticals production, the **Bioprocess Engineering group**, headed by Professor Udo Reichl, studies key aspects of the cell culture-based production of virus particles, viral vectors and other biologicals. Virus production processes are currently seeing a strong increase in market share due to the emergence of new diseases and a steady increase in general demand. This concerns, in particular, the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) pandemic. Furthermore, the growing use of viral vectors in gene therapy, and promising options for viral therapy to cure certain types of cancer or autoimmune diseases demand significant efforts. As in previous years, influenza virus propagation in animal and human cell lines is

considered a model system in bioprocess development due to its enormous relevance as a respiratory pathogen, the high complexity involved in virus-host cell interactions, its frequent mutations including gene reassortment, and options for using influenza virus-derived defective interfering particles (DIPs) as a new class of antivirals.

The group combines the expertise of five teams covering different aspects of biologics production, analytics and modeling. The **Upstream Processing team** (PD. Dr. Yvonne Genzel) focuses on virus and viral vector production processes. Therefore, the propagation of influenza virus, Zika virus, attenuated yellow fever virus, modified vaccinia Ankara virus and various other viruses is characterized in adherent and suspension cell lines. Studies involve the design and optimization of processes performed in stirred and orbital shaken bioreactors, hollow fiber-based systems and disposable units. In addition, advanced cultivation strategies using online sensors and cell retention devices are being developed to intensify manufacturing processes and further increase productivity. Details of virus-host cell interactions are studied by the **Molecular Biology team** (Dr.-Ing. Sascha Kupke) to identify bottlenecks in virus replication and to develop new strategies for antiviral treatment. Virus dynamics are investigated on the single cell and cell population level by a combination of classical virus quantification assays and state-of-the-art methods such as quantitative real-time PCR and imaging cytometry. The experimental data obtained from both groups are used by the **Mathematical Modeling team** (Prof. Udo Reichl) to elucidate fundamentals of cell growth, metabolism and virus replication. Multiscale models are established to simulate the spreading of infections and the accumulation of viruses in bioreactors starting from the single cell level. With a focus on proteomics, glycomics and glycoproteomics, the **Bio/Process Analytics**

team (Dr. Erdmann Rapp) is developing a comprehensive set of bioanalytical tools for the in-depth analysis of protein expression and posttranslational modifications of proteins. Finally, the **Synthetic Biotechnology team** (Dr. Thomas Rexer) is concerned with the development of enzyme-based process platforms for efficient *in-vitro* glycosylation of proteins and peptides and the establishment of technologies for the synthesis of nucleotide sugars and human milk oligosaccharides.

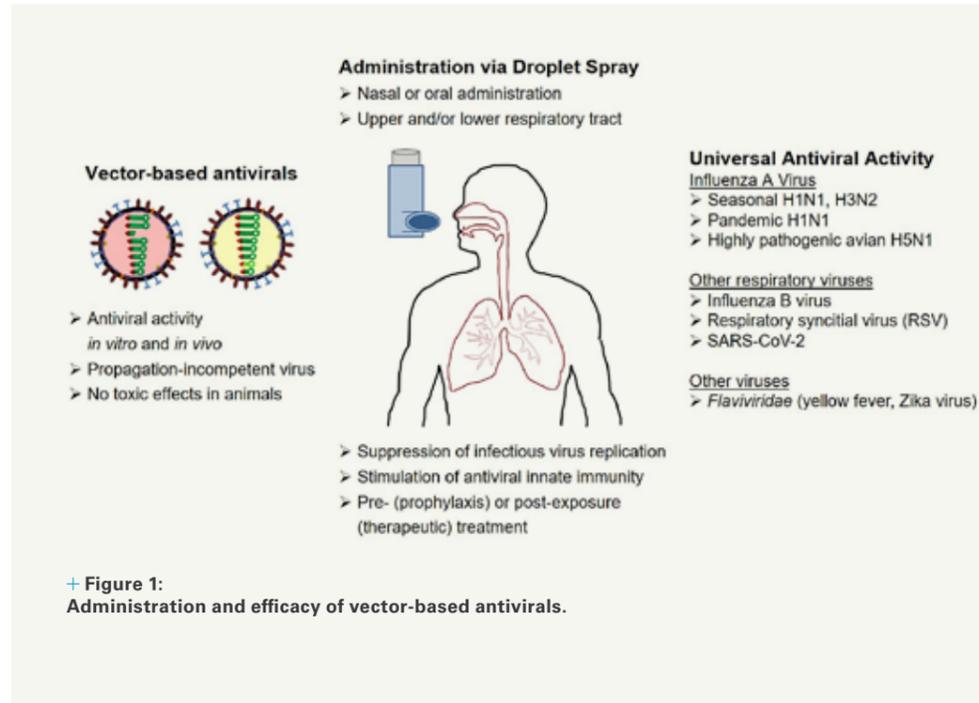
Over the last years, the Upstream Processing team has continued its efforts towards process intensification and process integration by optimizing perfusion strategies for high cell density cultures, and by exploring options for cell and virus retention using hollow-fibers, settlers and acoustic filters. With the recent challenges of the SARS-CoV-2 pandemic, collaborations with several research groups and commercial partners have been initiated to tackle various aspects of vaccine development. The spin-off project “ContiVir” was initiated successfully to continue the development of a manufacturing platform for viral gene therapy vectors within a two-year funded “EXIST-Transfer of Research” project. Furthermore, processes have been established for high-yield DIP production. This involves not only conventional influenza A virus-derived DIPs, which are characterized by large deletions in their RNA segments, but also a novel interfering particle, OP7, which contains various nucleotide substitutions in its segment 7, that was recently discovered by our group. To test hypotheses regarding the DIP interference mechanism, multiscale models are being developed that quantitatively describe DIP and standard virus replication dynamics for a wide range of infection conditions in cell cultures and bioreactors. Our efforts in synthetic biotechnology have resulted not only in the filing of a patent family covering enzyme-based processes for the synthesis of various

sugars and glycans, but also in the generation of various forms of glycosylated coronavirus Spike proteins for vaccine development. Based on this, another EXIST research transfer grant covering over 0.9 Mio € could be raised from the Federal Ministry for Economics and Climate Action. The start-up “eversyn” will use its proprietary, cost-efficient and highly scalable technology for the synthesis of nucleotide sugars and human milk oligosaccharides that are in high demand in the food and pharma industry. Finally, the Bio/Process Analytics team has further extended its portfolio of glycoanalytical methods for mass spectrometry-based peptide- and glycopeptide-mapping that are utilized not only for the in-depth analysis of viral antigens and synthetic glycosylated peptides but also in numerous collaborations in basic research, i.e. a project focusing on congenital disorders of glycosylation (CDG) within the scope of the DFG research unit FOR 2509: “The Concert of Dolichol-Based Glycosylation - from Molecules to Disease Models”.

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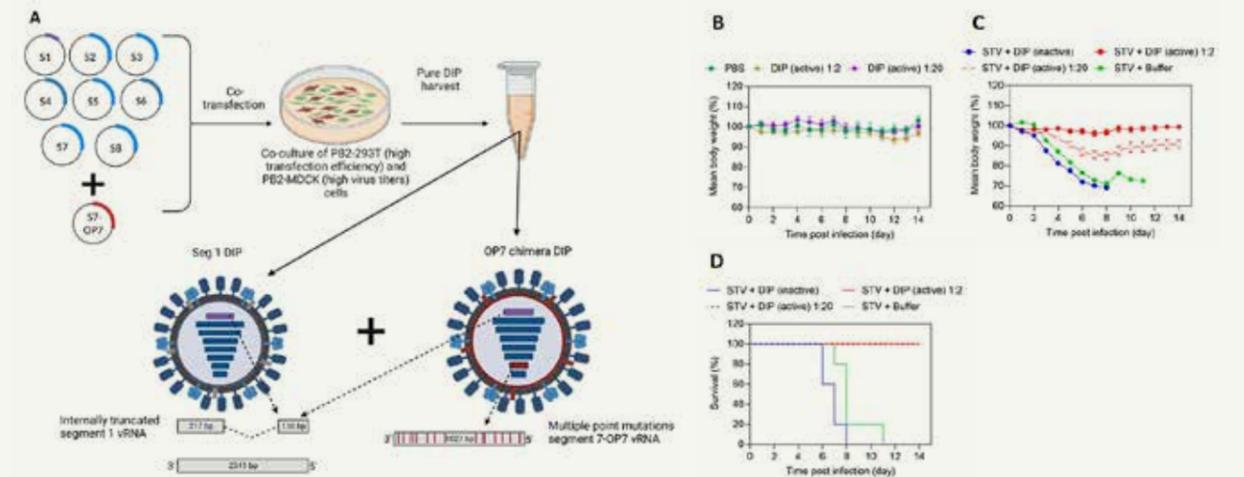


Broad-Spectrum Vector-Based Antiviral Agents

Influenza viruses cause respiratory disease and are considered a major human pathogen. As a result of their fast adaptability, influenza virus epidemics occur every year. These epidemics can cause up to five million cases of severe illness (especially in susceptible individuals) and up to 650,000 deaths worldwide. Of the four different genera, only the major human pathogen influenza A virus (IAV) can occasionally cause severe pandemics. In the last 100 or so years, four pandemic IAV outbreaks have occurred. Of these, the “Spanish influenza” (1918) was the most severe, claiming about 50 million lives worldwide. Pandemics happen when novel IAV strains emerge. These are able to infect people easily and spread efficiently from person to person in a sustained way. Prime candidates for a devastating pandemic are highly pathogenic avian IAV strains that can sporadically infect humans. Yet, in general, human-to-human transmissions are very rare. Currently, it is unknown whether these strains are ever able to adapt and cause a pandemic. Countermeasures to minimize influenza infections include vaccination and the use of antiviral small molecule drugs like oseltamivir and zanamivir. However, currently available vaccines have to be updated annually, and the development and production of a new vaccine for every season is a cumbersome and time-consuming process. In addition, some circulating human influenza virus strains have acquired resistance against commonly used antivirals. Clearly, new broadly acting treatment options would be highly welcome.

Recently, new vector-based vaccines have been approved for human use, including vaccines to protect against SARS-CoV-2 or Ebola virus infection. Such vaccines comprise genetically engineered viruses that are unable to propagate and cause disease. Instead, the transgenic and defective viruses lead, upon infection at the site of vaccination, to the expression of viral antigens. This way, the body’s immune response can mount long-lived protection against the target natural virus infection.

In our research team, we focus on a similar approach, namely vector-based antivirals that are based on naturally occurring defective interfering particles (DIPs) of IAV. DIPs lack an essential part of their viral genome, which is the origin of their defect to propagate upon infection. Interestingly, DIPs inhibit infectious, wild-type virus replication in a co-infection scenario. In such a co-infection, DIP replication withdraws and depletes cellular and viral resources, ultimately leading to the suppression of infectious virus dissemination. As a result, DIPs have been suggested as potent antiviral agents. Moreover, a given IAV DIP can inhibit a variety of IAV subtypes, including contemporary seasonal and pandemic strains and even highly pathogenic avian strains. Further, DIP infections stimulate the body’s innate immune response, an antiviral response that counteracts virus spread. Surprisingly, we have been able to show that this stimulation even leads to the suppression of the replication of foreign, non-homologous viruses including SARS-CoV-2 [1]. Therefore, we are



attempting to develop IAV DIP-derived vectors as a universal antiviral agent for treating the influenza disease and other respiratory viral infections (Figure 1).

The vector-based antivirals are generated using animal cell cultures. Here, the cells are transfected with tailored, genetically engineered viral DNA sequences. Afterwards, using the provided blueprint, the cells will start to synthesize progeny defective viral genomes and viral proteins. The viral components will then eventually self-assemble at the cell membrane to form “artificial” defective viral particles, or vector-based antivirals, that are released from the cells (Figure 2). The viral DNA sequences used for transfection are genetically modified, such that the safety, immunogenicity, and antiviral efficacy can be continuously improved. For instance, we used sequences from a novel IAV DIP (OP7) with an as-yet-unknown genetic structure, coincidentally discovered in our laboratory [2] in single-cell IAV infection experiments [3]. Intriguingly, OP7 showed superior antiviral efficacy compared to conventional DIPs [1, 4, 5]. In addition, we developed a high-yield cell culture-based production process in a laboratory-scale bioreactor, and purified our vector-based antivirals with a state-of-the-art chromatographic process [6]. Finally, we tested manufactured vector-based antivirals in mice experiments. First of all, no apparent toxic effects were observed in mice treated with vector-based antivirals. Further, all mice (100%) treated with an otherwise lethal dose of IAV were rescued from death upon co-administration with our vector-based antivirals (Figure 2), demonstrating their remarkable antiviral potential [4, 5].

However, the transfer of research findings into clinical application is typically very expensive and not easily accessible for research institutions. Therefore, we are currently setting up a good manufacturing practice (GMP) production process

(in collaboration with the Fraunhofer Institute for Toxicology and Experimental Medicine, Hanover/Brunswick), which is required for the initiation of safety studies and clinical trials in humans. By doing this, we expect significantly reduced cost risks and development times, with the aim of attracting start-ups or pharmaceutical companies for out-licensing of our patents. In addition, consultation with the German federal authority, the Paul Ehrlich Institute (PEI), will be conducted to ensure that regulatory matters relating to the production and clinical testing of this new class of antivirals intended for oral use are addressed correctly. | **Dr.-Ing. Sascha Kupke**

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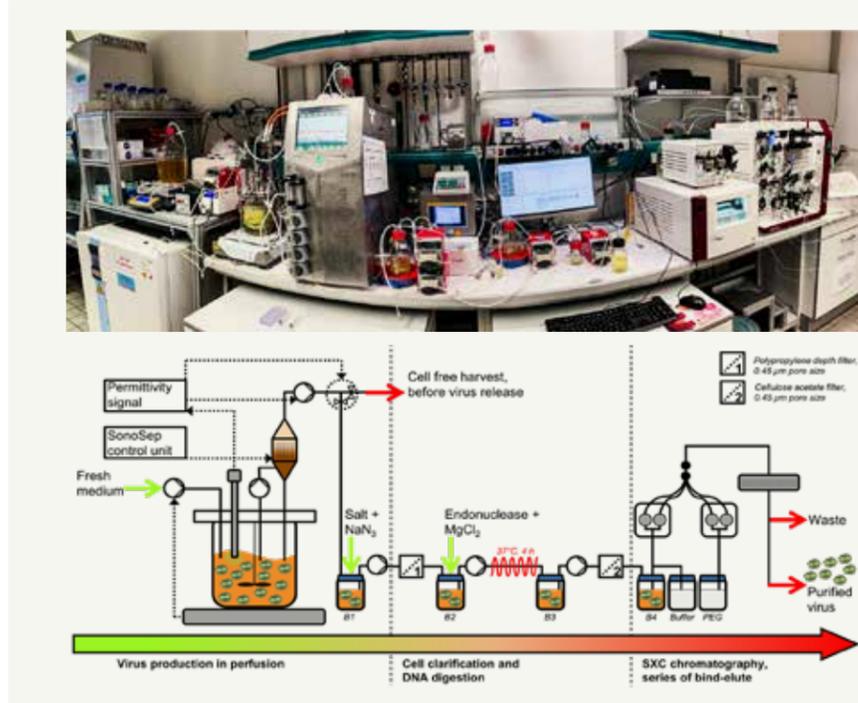
Patents: EP18159908 and EP21157812.5

Author **Dr.-Ing. Sascha Kupke**

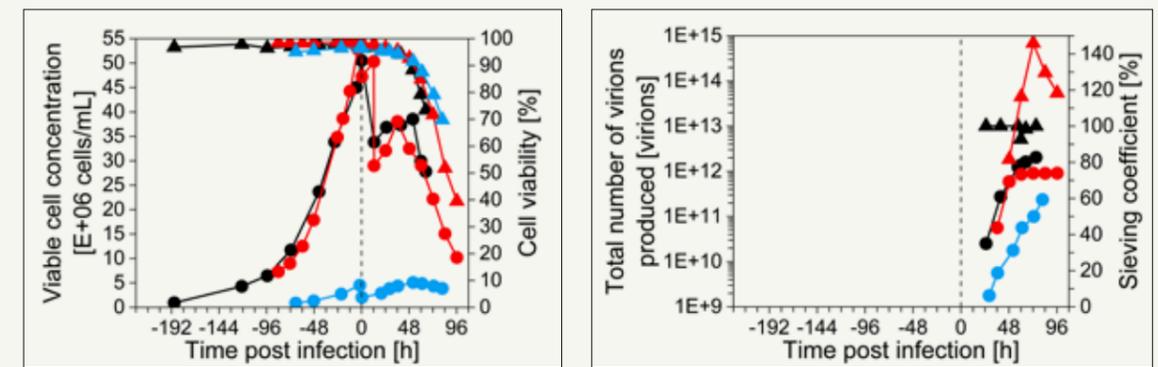
Sascha Kupke studied Biotechnology at the Technical University Berlin and Dongseo University Busan, South Korea (dual degree program). He graduated (Dipl.-Ing. and M.Eng.) in 2012. In the same year, he joined the Bioprocess Engineering Group at the Max Planck Institute for Dynamics of Complex Technical Systems (Magdeburg) as a Ph.D. candidate, working with single-cell analyses of IAV. Since 2020, he has led the Molecular Biology team of the Bioprocess Engineering group, focusing on applied research on IAV-derived defective interfering particles for antiviral treatment.

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+ Figure 1: End-to-end production of Modified Vaccinia virus Ankara (MVA): Integrated 1 L bioreactor perfusion cultivation, continuous harvesting, clarification and DNA digestion, followed by semi-continuous purification running on a laboratory bench^[2]. MVA is approved as a vaccine for smallpox. In addition, it is being considered for a monkey pox vaccine, as a vector for viral vaccines (e.g. HIV) and for gene therapy applications.



+ Figure 2: MVA production in AGE1.CR.pIX cells in perfusion and in batch mode (1 L stirred tank bioreactor; chemically defined medium). (Left) Viable cell concentration (●) and cell viability (▲), (right) total number of infectious MVA particles produced (●) and recovery coefficient (from the acoustic settler filtration step) (▲). Black and red symbols: perfusion cultivation 1 and 2; blue symbols: average from three batch cultivations^[3].

End-to-End Next-Generation High Yield Viral Vector Production

Currently, gene therapy is seeing a huge revival. Many developments and innovations in basic and applied research have facilitated that therapeutic viruses and viral vectors are considered the next rising star blockbusters. This is demonstrated by an ever-increasing number of clinical studies that rely on viral vectors for therapeutic use, e.g. <https://clinicaltrials.gov/>. Moreover, these viral vectors can equally be used as a safe vehicle to present immunogenic antigens of highly pathogenic viruses, such as HIV, SARS-CoV-2 or Ebola virus, and thus deliver urgently needed vaccines. To ensure this acceleration in newly identified targets for critical health indications is reflected in a smooth transfer to clinical studies, manufacturing of all these candidate viral vectors at high yield and large scale will be needed. This also applies to gene and oncolytic therapy, where an extremely high infectious virus particle input per dose is required. The Upstream Processing Team therefore focuses on the development of next-generation, highly efficient and sustainable virus production processes with candidate viral vectors, to propose new solutions and to train knowledgeable scientists and engineers in virus production and purification technologies to handle upcoming demands. Therapeutic viruses are either viruses for gene therapy applications or for direct disease treatment, such as oncolytic viruses. Predicted needs of infectious virus material per dose are currently extremely high and, depending on the respective indication, treated patient groups can be very large. Thus, highly efficient production systems

and purification trains are needed for manufacturing processes to guarantee sufficient supply for clinical studies and, finally, clinical applications. With respect to gene therapy, the production of personalized small batches might also be important, and therefore the establishment of high-yield single-use platform technologies might play a key role. In order to address these needs, a process for the production of Modified Vaccinia virus Ankara (MVA) was previously established in our group^[1] and has now been further improved. MVA can be used as a vector in gene and cancer therapy or as vector for vaccine applications such as Ebola or HIV vaccines. Furthermore, it is a candidate virus for a monkey pox vaccine. MVA is a DNA virus and is very large (400–500 nm). Thus, it is not possible to use sterile filtration methods using 0.2 µm cut-off filters to ensure product safety. For all applications, infectious virus particles are needed to present the antigen of interest. The virus is attenuated and can infect most cells to present its antigen. However, it can only replicate efficiently in avian cells to high infectious viral vector titers. Because of its attenuation, handling of MVA is allowed at biosafety level 1 (BSL1). Attenuation has led to a significant loss of its viral genome, enabling a large capacity for the insertion of “genes of interest” compared to other viruses.

Over the last years, we have compared MVA production in an avian cell line (AGE1.CR.pIX) in shake flasks, in hollow fiber, orbital shaken and stirred tank bioreactors (STR) using various cultivation options. These included batch, fed-batch,

two-stage continuous, and different perfusion strategies. Eventually, we identified best results on virus yield and volumetric productivity for cultivation in perfusion mode^[2]. Compared to conventional batch production, this allowed increasing the cell concentration significantly while keeping a high cell-specific virus yield. As a result, up to 8×10^9 infectious virions/mL could be harvested. In a next step, we integrated virus purification directly into the perfusion process, to allow for the complete process running continuously and end-to-end on one of our laboratory benches^[3]. Therefore, virus production in a 1 L STR was directly coupled to continuous harvesting, digestion of host cell DNA and subsequent semi-continuous purification using steric exclusion chromatography (Figure 1). Cell retention via an acoustic settler and a medium dilution step at time of infection resulted in a maximum concentration of 37×10^6 infected cells/mL. Cell growth was monitored via a capacitance sensor and the perfusion rate was tightly controlled according to the needs of AGE1.CR.pIX cells. Infection resulted in a harvest of up to 2×10^{12} infectious MVA particles (Figure 2). Finally, the purification train set-up enabled an overall recovery of 50.5% and removal of host cell DNA below the required limits. A first academic techno-economic analysis demonstrated that, overall, the space-time-yield at the 1 L scale was increased by 600% in perfusion mode compared to batch cultivation with a possible cost reduction by a factor of 2.8. Accordingly, using our bioprocessing toolbox, the continuous production technology established could be a first step and a template for other next-generation virus manufacturing processes. In addition, it can serve as an important element for the set-up of a comprehensive platform knowledge base.

Currently, the Upstream Processing Team is collecting extensive process information for various virus-host cell combinations and cultivation modes. This includes the evaluation of

new technologies and process strategies for their benefit in virus manufacturing, such as single cell cloning and selection, the use of parallel-operated micro-bioreactors and orbital shaken bioreactors, the selection of media components and feeding strategies for boosting virus yields, and the identification of options for optimal membrane-based cell retention.

PD Dr. Yvonne Genzel

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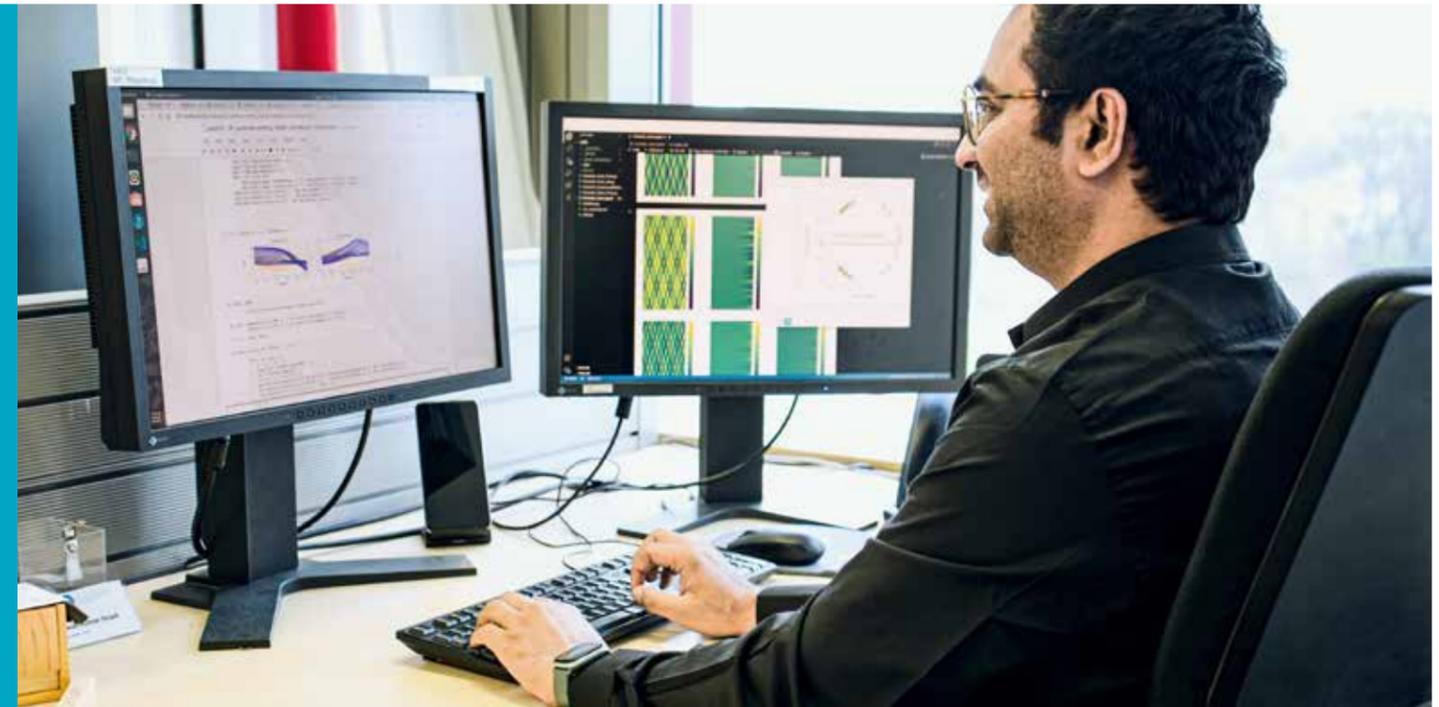
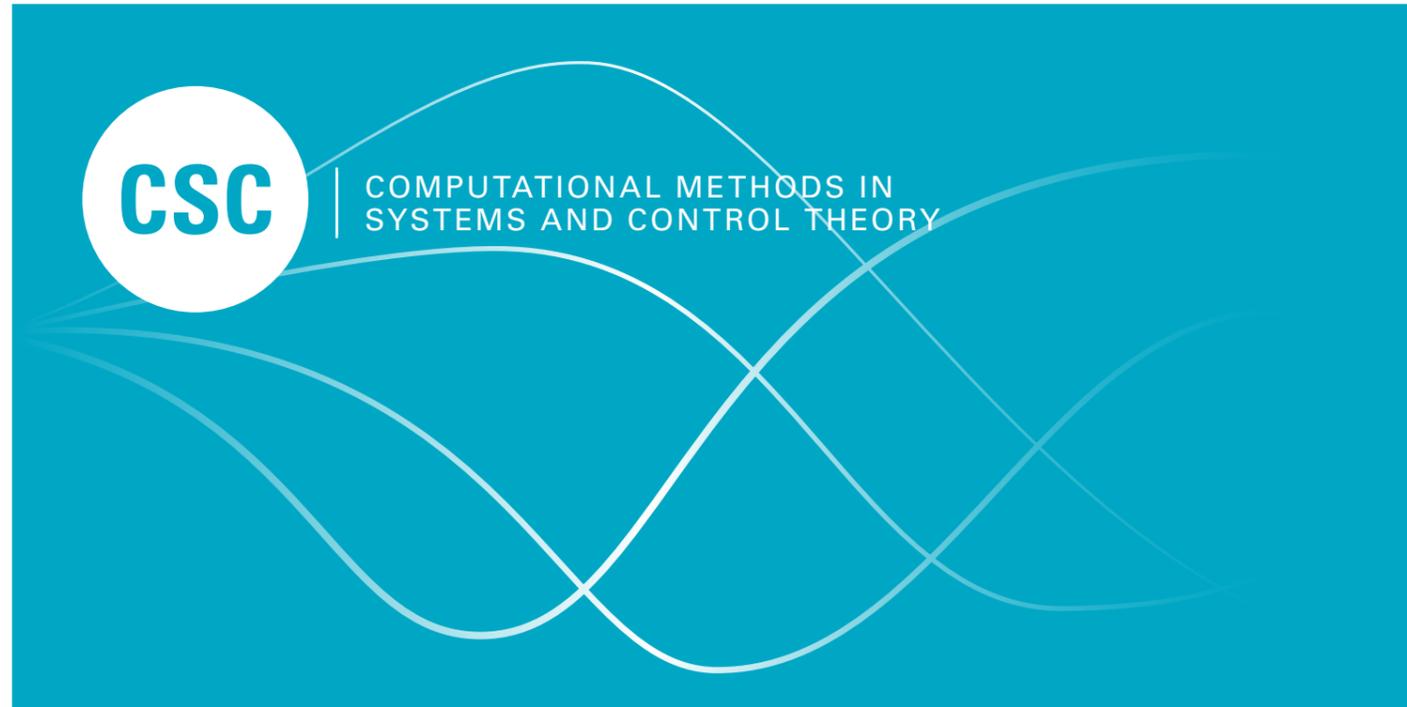
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Author PD Dr. Yvonne Genzel

Yvonne Genzel studied Technical Biology at the Technical University of Stuttgart and obtained her Ph.D. at the University of the Mediterranean, Marseille, France. In 2001, she joined the BPE group in Magdeburg, later leading the Upstream Processing Team. She received her habilitation from the OVGU in 2009. Her interest lies in process development and intensification for cell culture-based virus production. Training young scientists in these technologies with state-of-the-art equipment and direct industry-relevant virus host-cell systems and applications motivates her, with a vision of enabling next generation vaccine manufacturing.

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+ Computational Mathematician Dr. Pawan Goyal is developing algorithms for data-driven dynamical modeling as one of the core tasks of the CSC group toward scientific machine learning.

PROF. DR. PETER BENNER | DIRECTOR

The CSC group is concerned with modeling, simulation, optimization, control, inference, and uncertainty quantification of time-dependent problems from the sciences and engineering. CSC researchers employ mathematical ideas and concepts to develop new methods for in silico design or experiments for complex technical systems such as those investigated, for example, in the engineering departments at the MPI. Specifically, we consider efficient simulation – enabling this via reduced-order models – as well as optimal and feedback control of dynamical systems, i.e. of mathematical models described by systems of differential equations. Since 2020, we have strengthened our efforts on including machine learning into our research portfolio, in particular for the inference of mathematical models from data (as highlighted on the next pages). The areas of application range from chemical and biotechnological processes and electro-magnetic devices to energy networks and materials discovery. Our workflow often includes sophisticated programming strategies for modern computer architectures and clusters, such as hardware accelerators like GPUs, as well as energy-awareness in the algorithm design. We use different hardware platforms, including our Linux cluster, *mechthild*^[1], with 2000+ cores, and several GPU-powered workstations.

CSC Teams

Since 2015, the CSC structure had comprised 6 teams, which changed to 7 in 2021: **Model Order Reduction (MOR)** (headed by L. Feng) dealing with mathematical methods to algorithmically reduce the number of degrees of freedom in mathematical models in order to accelerate their simulation, facilitate their optimization, enable control design, and quantify uncertainties. The **Computer Aided Control System Design (CACSD)** team (J. Heiland, also an assistant professor at OVGU) considers computational methods for control systems. The **Simulation of Energy Networks (SES)** team (S. Grundel) focuses on the modeling and numerical simulation of energy transportation networks. Recently, transport of hydrogen in gas networks has become a new research focus of SES. Efficient **Numerical Linear and Multilinear Algebra (NLMA)** techniques percolate almost every aspect of CSC research. The NLMA team (P. Benner) deals with eigenvalue problems, preconditioning and tensor techniques, as well as the numerical solution of (Lyapunov, Sylvester, Riccati) matrix equations. The latter was in the focus of the **Matrix Equations (ME)** team, while efficiently implementing numerical algorithms on modern computing platforms was the task of the **Scientific Computing (SC)** team, both led by J. Saak. In order to adapt to the recent focus on data science and machine learning, the ME team was partially included into NMLA and partially into the new team **Data, Infrastructure,**

Software & Computing (DISC), led by J. Saak, that also absorbed the SC team. Moreover, we launched the new teams **Physics-Enhanced Machine Learning (PML)**, led by P. K. Goyal, and **Structured Dynamical Systems (SDS)**, led by I. Pontes Duff.

Highlights and Developments in 2021/22

In addition to the research trends highlighted in the first paragraph, our activities in Research Data Management following the FAIR principles have become increasingly visible through our involvement as co-applicants in the NFDI (National Research Data Infrastructure) consortia **NFDI4CAT** (Digital Catalysis, 2020-2025) and **MaRDI** (Mathematical Research Data Initiative, 2021-2026).

The Sars CoV-2 pandemic continued to pose challenges for our group. We pursued several COVID-19-related projects, including the development of optimal testing strategies for medical care facilities together with University Hospital Magdeburg and the Children's and Youth Psychiatric Clinic Magdeburg as well as the development of age-aware compartment models for optimizing contact reduction and vaccination schedules.

Another challenge arose from Russia's war in Ukraine. Due to our strong links to the National Academy of Sciences of Ukraine and in particular its Institute for Applied Mathematics

and Mechanics in Sloviansk, we integrated three scientists from the Sloviansk area into the CSC department and established further links to another NASU institute with the help of the EIRENE program of the Max Planck Society.

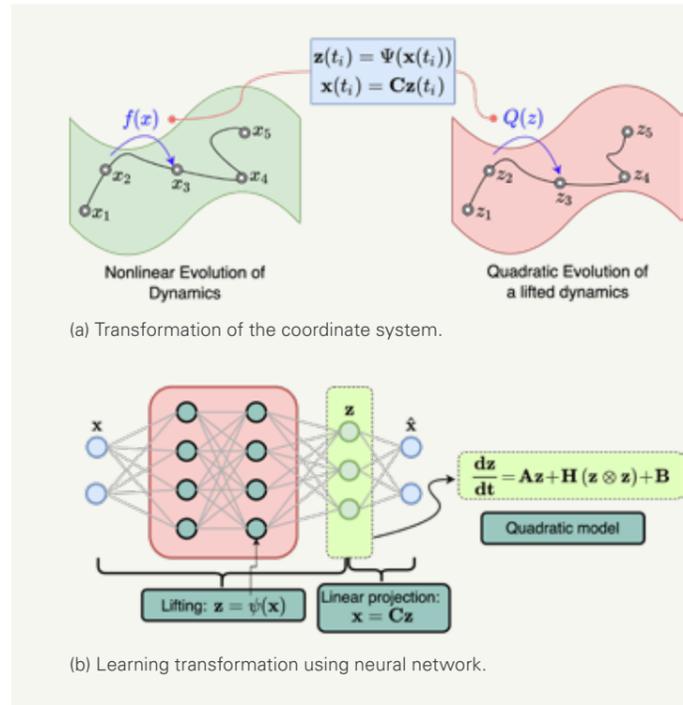
A particular highlight was the first group retreat after the COVID-19 outbreak. This was held at the Max Planck Society's own Ringberg Castle in Southern Bavaria in February 2022. It was a great experience to be able to mingle, exchange research ideas in lively personal conversations, and enjoy the splendid location together after two years of social distancing!

[1] Named after "Mechthild von Magdeburg" (c.1207- c.1282/94), a Beguine and the first mystic to write in German.

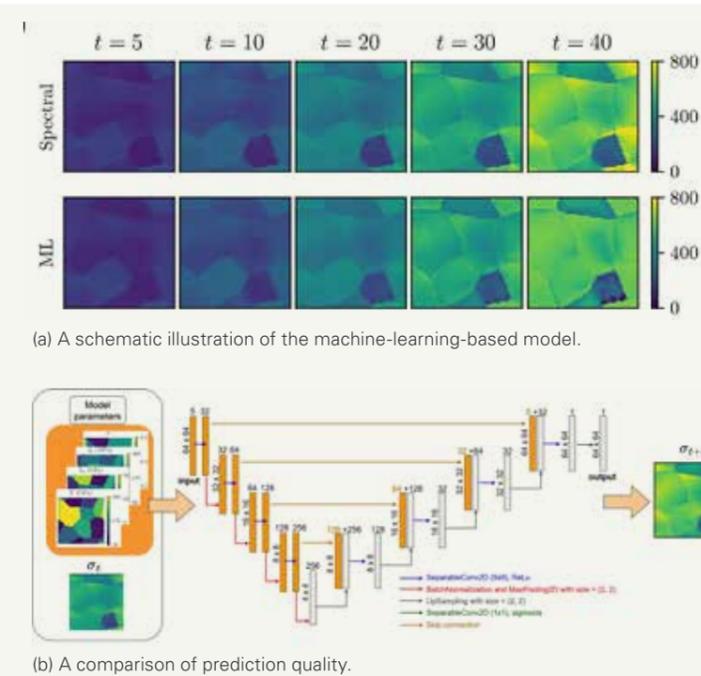
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+ Figure 1: Lifting-principles allow smooth nonlinear dynamical systems to be rewritten as quadratic systems in suitable coordinate systems which capture the dynamics of the original nonlinear system exactly. We focus on learning such a coordinate system using data and tailoring auto-encoder design as shown in (b) to achieve the goal, which can ease the engineering design process.



+ Figure 2: The schematic illustration of the machine-learning-based model for predicting the history-dependent local von Mises stress. In the figure, E : Young's modulus, μ : Poisson ratio, ξ_0 : initial flow resistance, h_0 : initial isotropic hardening, and σ : von Mises stress. We construct a surrogate model of stress fields for viscoplastic polycrystalline materials using U-Net as shown in (a), which predicts von Mises stress field 500 times faster than conventional spectral solvers, see (b).

Machine Learning for Dynamical Systems

Introduction

Understanding physical phenomena and dynamic behavior via data-driven mathematical models has been an active research field for centuries. For example, J. Kepler established his three laws of planetary motion in the 17th century by analyzing the astronomical observations of T. Brahe. Mathematical modeling is essential for the discovery of fundamental laws and the execution of engineering studies such as process control, and forecasting. Traditional modeling approaches are based on known physical laws and empirical knowledge. However, this is intractable for complex systems, e.g., robot dynamics, complex biochemical reactions, or downstream processes for vaccine production, to name just a few applications. Using data-driven methods leveraging artificial intelligence advancements, the aim is to build dynamic models for complex processes to uncover the underlying physics and streamline engineering design procedures and digital twinning.

Discovering physical laws

The research frontier of discovering physical laws from data has demonstrated its potential in history. It still remains highly relevant to scientists and researchers to better understand and design physical processes. An essential ingredient is to have an analytic mathematical expression describing the underlying dynamics, which experts can interpret. With these goals, symbolic and sparse regression techniques have shown their

versatility. In the CSC department, we have actively pushed the frontier by developing advanced methodologies^[1]. By leveraging advances in machine learning and deep learning, we have introduced approaches dealing with noisy data, which are inevitable when collecting data in labs. We explore this research frontier further in collaborations with Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany, to understand the interfacial problems in material science, aiming to improve the material design process and understand phase-field models.

Physics-enhanced surrogate modeling

Numerical simulations are the foundation of the engineering design process of complex systems. However, their complexity and high fidelity make the design process unacceptably slow and expensive. To alleviate the computational burden, we develop surrogate models of complex high-fidelity models so that they not only mimic the behavior of the complex systems but are also computationally efficient enough to query them during engineering design processes.

An intriguing approach to efficiently performing simulations for high-fidelity models is the construction of low-fidelity models. This can be achieved by projecting the high-fidelity models onto a low-dimensional manifold. In this context, we have explored a data-driven approach, known as operator inference (Oplnf), for building low-fidelity models using data collected from modeling design software. A key characteristic of Oplnf is how it

abstractly incorporates prior physical knowledge from high-fidelity systems to construct low-fidelity models, which is a step towards physics-informed learning. The CSC department has developed a number of methodologies for nonlinear and parametric systems based in this direction^[2]. In the future, we will keep studying this fascinating research field to enhance its predictive capacities and robustness for practical applications.

As an alternative strategy to accelerate the engineering design process, the CSC department has focused on identifying suitable coordinate systems, which can facilitate not only understanding but also the design process. For instance, the Fourier coordinate system can make the description of the heat equation simpler. In these contexts, we have developed the notion of learning quadratic embeddings for nonlinear dynamic models^[3]. It leverages the fact that nonlinear systems can be written as quadratic systems in appropriate coordinate systems, which are identified by neural networks as depicted in Figure 1.

Our attention has also been on surrogate operator learning, which can forecast dynamic behavior much faster than conventional methods. In such setups, neural network-based surrogates have demonstrated their success. We have brought these advancements to material science in collaboration with the material science department at Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany, led by Prof. Dierk Raabe. We have constructed surrogate models for stress fields in viscoplastic polycrystalline materials^[4], which can predict material behavior up to 500 times faster than classical techniques with high accuracy, see Figure 2.

Outlook

We have discussed our efforts toward advancing the research frontier of data-driven discovery and surrogate modeling of dynamical systems. We have closely collaborated with phys-

icists and engineers to translate these technologies to real-world applications. In the future, we will continue our efforts to develop cutting-edge methodologies by bringing artificial intelligence, dynamical systems, and physics together, and make a positive impact on the development of digital twin and engineering design cycles. | **Dr. Pawan K. Goyal**

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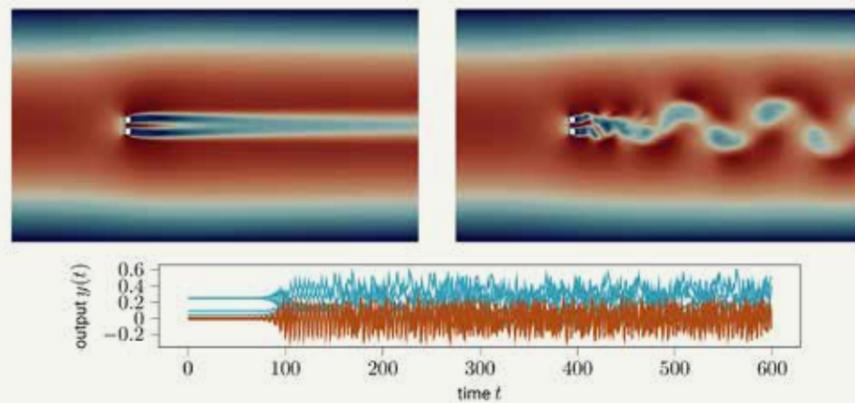
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Author Dr. Pawan Goyal

P.K. Goyal graduated from the Department of Engineering Design at the IIT Madras, Chennai, India, in 2013. He then joined the department of Prof. Peter Benner at the Max Planck Institute (MPI-DCTS), Magdeburg, Germany, for his Ph.D. In 2018, he received his Ph.D. in Mathematics from Otto von Guericke University, Magdeburg. Since 2021, he has been the team leader of the "Physics Enhanced Machine Learning" team in the CSC Department. His primary research interests include scientific machine learning, data-driven surrogate modeling, and physics-informed learning.

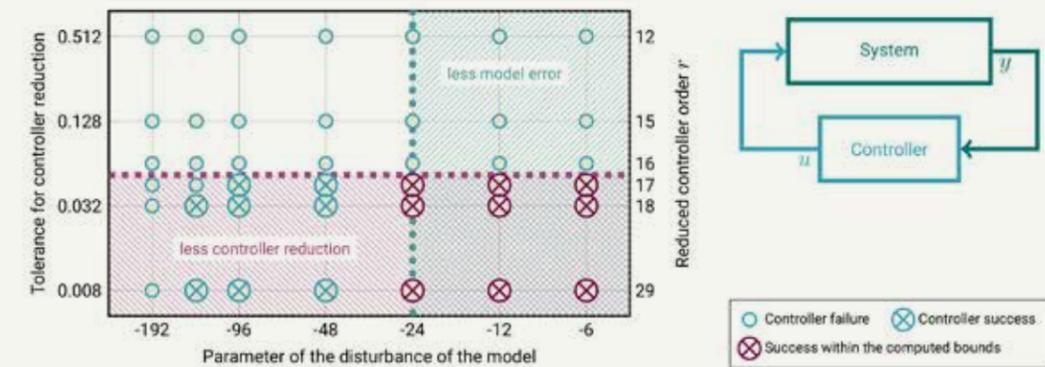
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+ Figure 1:

A snapshot of the desired steady state, a snapshot of the more realistic state without controls applied, and a measured signal that illustrates the fluidic behavior of the flow over time in the uncontrolled regime as it is attained after a short initial phase where deviations are hardly visible.



+ Figure 2:

Illustration of the performance map of our controller design for the flow example in Figure 1. Hereby, we verify the theoretical error bounds by simulating the controlled system for different reduced order models of the controller and for increasingly large perturbations of the model itself.

Robust Control of Complex Systems

Introduction

Once a mathematical model works for accurately predicting the behavior of a dynamical system, we will start thinking about using the model to actually control the system. By control, we mean observing states y of the system and influencing it accordingly via inputs u so that its state follows a desired behavior. The scheme of such an output feedback control is sketched in Figure 2.

Initiated by Kalman's groundbreaking works in the 1960s, mathematical control theory has had widespread and successful use, with the NASA Apollo mission as a prominent example.

In the context of control, possible but unavoidable discrepancies between the model and the system can be harmful in two respects. Firstly, the computed outcomes may inaccurately reflect the system behavior; secondly, the smallest modeling errors may severely deceive the control design and even cause a total failure.

Robust Control

In order to avoid failures in the possible presence of unknown errors in the models, the idea of robust control has been developed. The basic principle is that a computed control law must work not only for the model at hand but also for models that are slightly different.

Basic ideas of robust control, often denoted by H_∞ -control, have been investigated since the 1960s but reached a new level in the late 1980s when a state space formulation (cp. [1]) was developed that made the design feasible in numerical simulations. With the establishment of the theory in infinite dimensions and with decisive algorithmic advances for the closely related, performant, but not necessarily robust *linear-quadratic* controller design, all prerequisites were available to bring H_∞ -controller design to large-scale simulations.

In our work, we developed a numerical method, see [2], that can efficiently solve the large quadratic matrix valued equations as it is needed to design robust controllers. In view of efficient implementations, it is desirable to include model order reduction at least for the part that computes the controls. Therefore, we have combined error estimates on model reduction with estimates on modeling errors into general computable estimates (see [3]) to efficiently control simulations of incompressible flows. In order to be in line with the theory in infinite dimensions, that is with the model before it was turned into the simulation code, we have investigated relevant modeling errors in the Navier-Stokes equations directly; cp. [4].

Simulation Example

To evaluate the performance of our numerical methods for both the solution of the relevant matrix equations and the estimates that would guarantee the performance of the

controller, we considered the flow past a double cylinder. The regime was chosen such that – without control action – the flow would soon enter the state of periodic vortex shedding. In our setup, we modeled our controls to induce a rotation of the cylinders to avoid the switch from the quasi steady-state to the natural shedding of vortices.

Apart from providing control laws that kept the flow in the desired state, we showed that our estimates can predict how much modeling error, considering both model reduction error and errors in the linearization, can be admitted until the controller will fail.

Perspectives

So far, we can accommodate model errors that arise from a model order reduction or from inaccurate linearizations. Another error source that should be included is the discretization error. While qualitative results are available and while our work on the infinite dimensional model implies the required general consistency, for a practical realization we would need quantitative estimates on these source of errors. If this can be achieved, from some particular perspectives, the research on using H_∞ -controller design in numerical simulations will be almost complete. At the same time, we will work on algorithmic advances and example simulations beyond fluid flow applications. | Jun.-Prof. Dr. Jan Heiland

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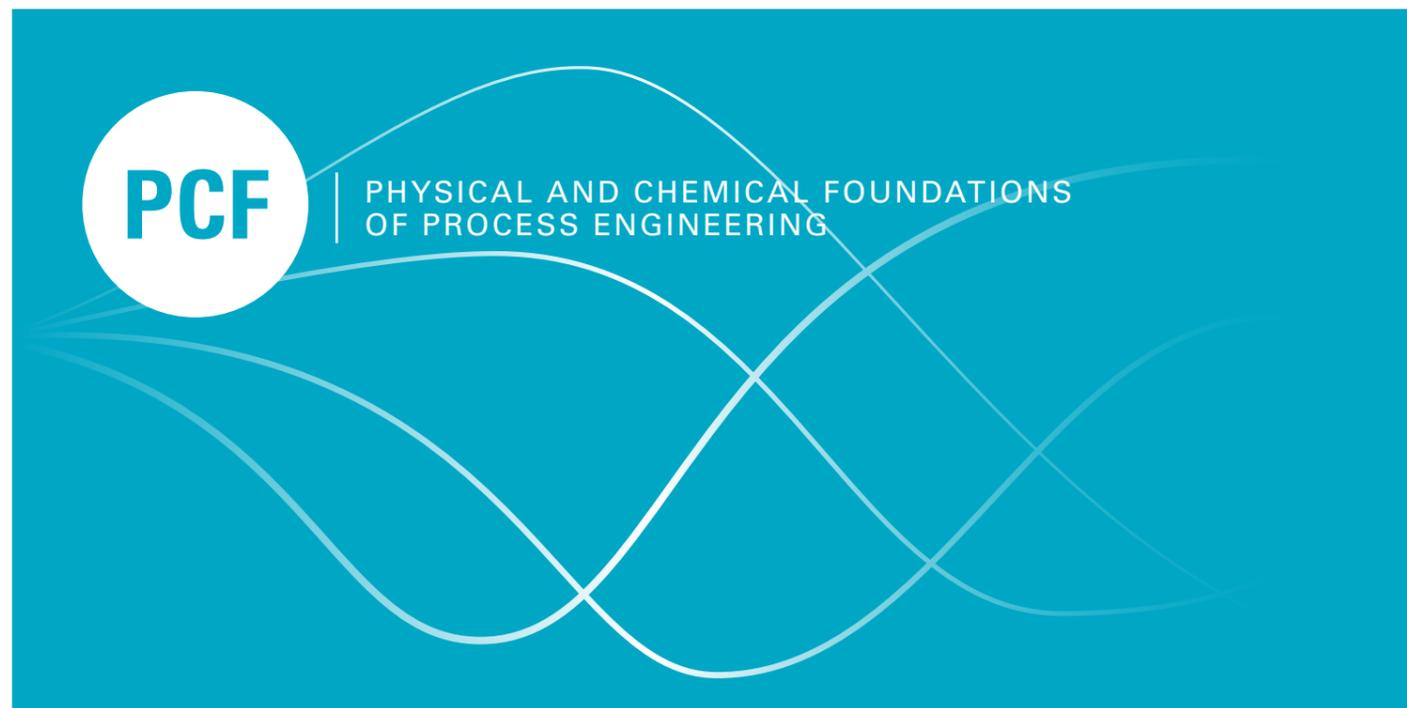
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Author Jun.-Prof. Dr. Jan Heiland

Jan Heiland graduated from the TU Berlin in 2009. After a short period working for Bombardier Transportation, he started a Ph.D. project at TU Berlin which he defended successfully in 2014. Since then, he has been a researcher and team leader at the MPI Magdeburg. In 2018, he was appointed Junior Professor at Otto von Guericke University of Magdeburg, and in 2021 became temporary full professor for data-driven design of dynamical systems at the FAU Erlangen/Nuremberg. Jan Heiland's research interests include system and control theory and robust control, differential algebraic equations, infinite dimensional systems, model reduction, and design and simulation of control systems.

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+ Chemical Engineer Dr. Peter Schulze is adjusting the air flow at the pilot plant for carbon dioxide direct air capture (CODA project).

PROF. DR.-ING. ANDREAS SEIDEL-MORGENSTERN |
DIRECTOR

+ To tackle the enormous global problems that we are facing, there is an urgent need to change our energy and feedstock bases. This requires the development of new transformation concepts which efficiently exploit dedicated chemical reactions, combined with efficient separation processes.

The Physical and Chemical Foundations of Process Engineering (PCF) group seeks to contribute towards isolating and purifying certain components or fractions from renewable resources that can be utilized as reactants in subsequent synthesis reactions.

We are attempting to isolate lignin from black liquor originating from wood processing. Recently, together with other partners, we successfully completed the European project UNRAVEL (UNique Refinery Approach to Valorise European Lignocellulosics). In contrast to possible depolymerization of the large lignin molecules to synthesize small aromatic bulk chemicals, we contributed to the development of sequential fractionation methods capable of generating well-defined low and high molecular weight lignin fractions, which can be a substitute for fossil resources in the materials sector.

Further, the PCF group is searching for ways to improve the efficiency of extracting valuable natural products from

plants. The research is particularly focused on developing efficient, continuously operating countercurrent extraction processes combined with purification techniques. Over the last two years, we have studied crystallization and chromatography based isolation of certain ingredients of saffron (extracted from *Crocus sativus*) and curcumin (extracted from *Curcuma longa*). We have also continued our activities to improve the provision of artemisinin (key ingredient in potent anti-malaria drugs) from *Artemisia annua L.*

Chemical reaction engineering oriented activities were focused on studying the homogeneously catalyzed hydroformylation reactions of transforming long-chain olefins available from renewable resources into valuable aldehydes. This research was imbedded in the larger DFG-funded SFB initiative InPROMPT and carried out together with colleagues from TU Berlin, TU Dortmund, and several other MPI and OVGU groups.

Currently, the PCF group is conducting theoretical and experimental studies on the potential of a forced periodic operation of continuous processes. For this, reactors and separation units are exposed to forced modulations of certain operating parameters, such as inlet concentrations and flow rates. In cooperation with Achim Kienle (OVGU), Menka Petkovska, and Daliborka Nikolic (both University of Belgrade) and supported by the DFG, we are studying the potential of forced fluctuations of the inlet composition of a catalytic reactor designed to produce methanol at elevated pressure from green hydrogen, CO₂ (available in waste streams and in the air), and CO (see pages 38-39, contribution by Lothar Kaps and Wieland Kortuz).

Exploiting CO₂ captured preferably from exhausts of industrial processes within a new process to produce soda ash is the aim of the CODA (Carbon-negative sODA ash) project. It was launched successfully in cooperation with the soda plant of CIECH Soda Deutschland in Staßfurt and is funded by the BMBF (see pages 36-37, contribution by Peter Schulze and Maria Gutierrez).

Over the last two years, our research devoted to isolating optically pure organic molecules (enantiomers) out of racemic mixtures has continued in different directions. For example, the PCF group has contributed to this important field for the pharmaceutical industry by developing and applying dedicated crystallization-based and chromatographic processes within the European project CORE (COntinuous REsolution of Chiral Components). Significant progress has been achieved in demonstrating the great potential of applying a conically shaped fluidized bed crystallizer. To exploit the unwanted counter-enantiomers, efficient enzymatic racemization in combination with recycling steps has been successfully tested.

Unfortunately, the long-lasting coronavirus crisis was a significant obstacle during the period of this report. It caused delays in finalizing novel experimental set-ups and acquiring experimental results. It also prevented us meeting with other scientists at conferences in order to discuss research results. Numerous online platforms helped us to stay in contact and exchange ideas. However, we all felt that this was not the same as discussing our research face to face. The cancellation of conferences was most disappointing for Heike Lorenz, the organizer of the International Symposium

on Industrial Crystallization (ISIC) which takes place only every three years and is the major international meeting in the field. After shifting the initially planned date, she set up a complete program twice with her committee. Finally, ISIC-21 was held very successfully online from August 30 to September 2, 2021.

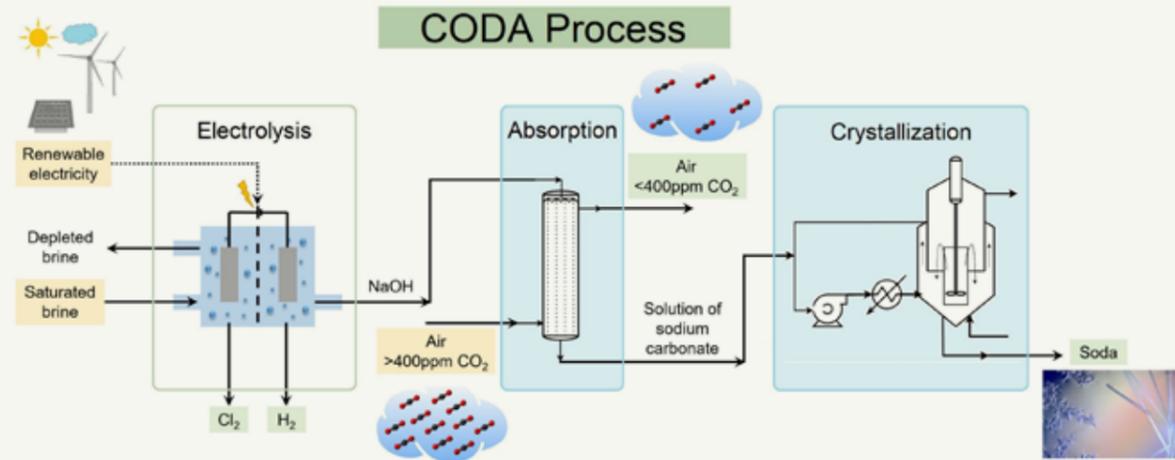
We are very happy that 2022 brought us opportunities to attend national and international meetings once again. These were particularly welcomed by our young colleagues and used efficiently to establish new personal contacts.

During the period of this report, the members of the PCF group published a significant number of research papers describing their research results. We also contributed towards finalizing a larger book project summarizing the results of the InPROMPT project.

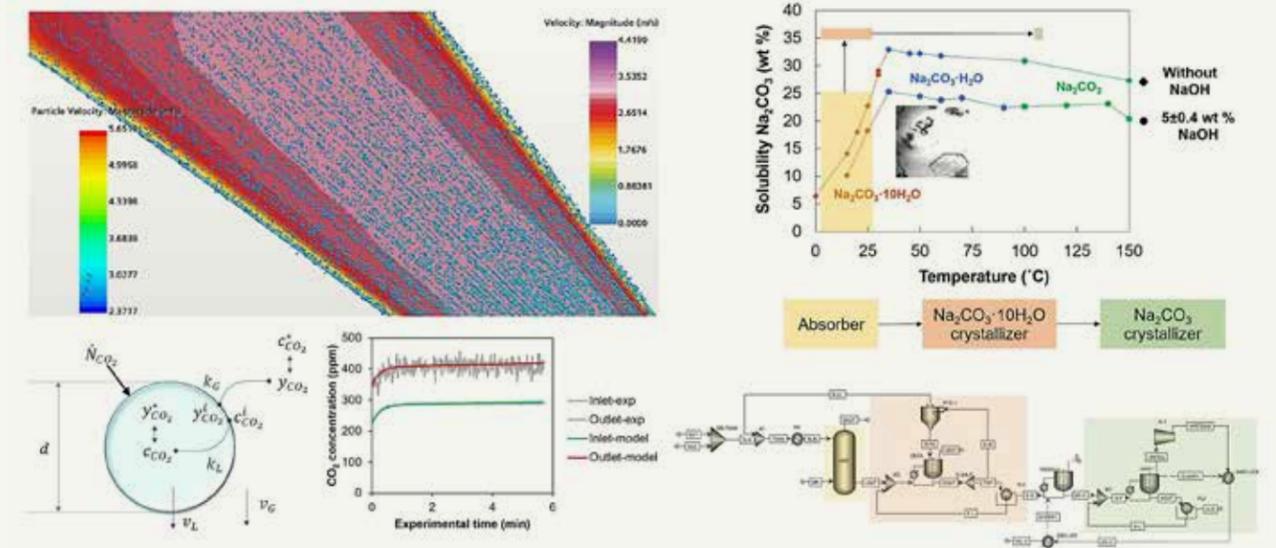
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+ Figure 1: Carbon-negative sODA ash production concept: absorption and crystallization are studied at MPI.



+ Figure 2: Mono-disperse droplet absorber simulations and experimental results (left) and sodium carbonate solubility diagram in the presence of NaOH for process conception (right).

Sustainable Production of Soda with CO₂ from Air

Although the development of the chemical industry has driven economic growth, traditional industries producing commodity chemicals have diverged from the United Nations' Sustainable Development Goals. High-energy requirements generating large greenhouse emissions and reliability on fossil-based feedstock are among the problems of large-scale manufacturing processes. For example, despite optimization efforts, the Solvay process used for more than 150 years to produce soda ash (short: soda) emits around 0.5 tons of CO₂ per ton of product. The design of a sustainable process able to capture CO₂ directly from air while producing soda ash is the aim of the CODA (Carbon-negative sODA ash) project which is carried out by the PCF group in cooperation with the soda plant of CIECH Soda Deutschland in Staßfurt and funded by the BMBF (Figure 1, [1]).

Besides directly avoiding the emission of CO₂, the CODA process would remove around 0.4 tons of CO₂ per ton of soda by direct air capture. While the Solvay process requires the calcination of limestone at 850–1100°C to obtain the carbon dioxide and quicklime needed to produce soda ash, the CODA process would take CO₂ from the environment at ambient temperatures. The CO₂ from air would be absorbed in a sodium hydroxide solution obtained by electrolysis of rock salt brine using renewable electrical energy. Anhydrous sodium carbonate crystals would be obtained from

the carbonated solution out of the absorber at milder conditions (max. 150°C). Byproducts of the CODA process are hydrogen and chlorine, which could be sold in the market or be used to produce hydrochloric acid and process energy. At the end of the CODA project, a pilot plant (TLR5) will be built and tested in the soda plant of the industrial partner.

Carbon Dioxide Removal (CDR) methods that remove CO₂ directly from air play a major role in many mitigation scenarios aiming to achieve climate neutrality. However, CDR technologies face technical and economical limitations related to energy consumption and the cost of the collection process. The sustainability assessment of the CODA process can only be positive if the energy consumption of all processing stages is the minimum possible and renewable energy is consumed. Due to the small concentration of CO₂ in the atmosphere (~415 ppm), the amount of air required to be processed is very high (min. 575 m³ air/ kg soda). Therefore, the absorber design should seek to minimize the pressure drop and the energy required to move the air.

Our aim is to design an absorber able to minimize the energy consumption and capital investment in the CODA process. In the absorption process, CO₂ is transported in the gas phase to a gas-liquid interphase; then, CO₂ is solubilized and transported in the liquid phase, where it reacts with the hydroxide

ions in the solution [2]. Depending on the equipment (geometry) and operational conditions (velocities and concentrations), the phenomena controlling the absorption process can be the mass transfer or the reaction. We are currently studying the absorption in a small scale-pilot plant configuration using a Mono-Disperse Droplet Absorber (MDDA) (Figure 2, left). The MDDA minimizes the energy required to move the air (smaller pressure drop), saves capital costs associated with the packing used in traditional absorbers and tolerates possible crystallization of soda. Here, the determination of the surface area for mass transfer is required for process modeling and optimization. Currently we couple Computational Fluid Dynamics (CFD) with a model describing the kinetics, thermodynamics and mass transfer inside the absorber to describe the CO₂ capture in our pilot plant.

Parallel work on the CODA project is focused on identifying a suitable crystallization strategy to obtain soda ash. We

are experimentally studying the solid-liquid equilibria and crystallization kinetics of the decahydrate, monohydrate and anhydrate of sodium carbonate (Figure 2, right). Preliminary process flowsheet simulations have shown that the formation of decahydrate at ambient conditions after the absorption, followed by the crystallization of anhydrate, is a promising crystallization strategy from an energy consumption point of view. Future work should focus on optimizing the coupled processes and its operation under different weather scenarios, while keeping it "carbon-negative". | **Dr.-Ing. Peter Schulze, Dr.-Ing. Maria Gutierrez**

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Author Dr.-Ing. Peter Schulze

Peter Schulze joined the PCF group as a Ph.D. candidate in 2013 and defended his Ph.D. project "Lignin Separation from Ethanol Water Pulp Liquors" in 2018. He studied Chemical Engineering at OVG University Magdeburg and received his diploma in 2010. Currently, he is working as a Team Leader responsible for the BMBF funded project "CODA" and two projects on autothermal CO₂ Direct Air Capture (DAC) in cooperation with the Arizona State University in the US.

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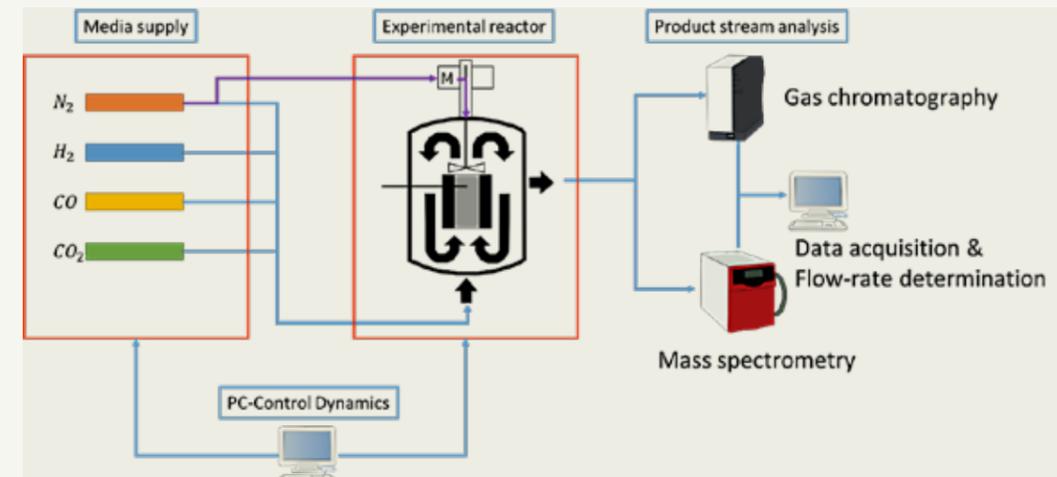
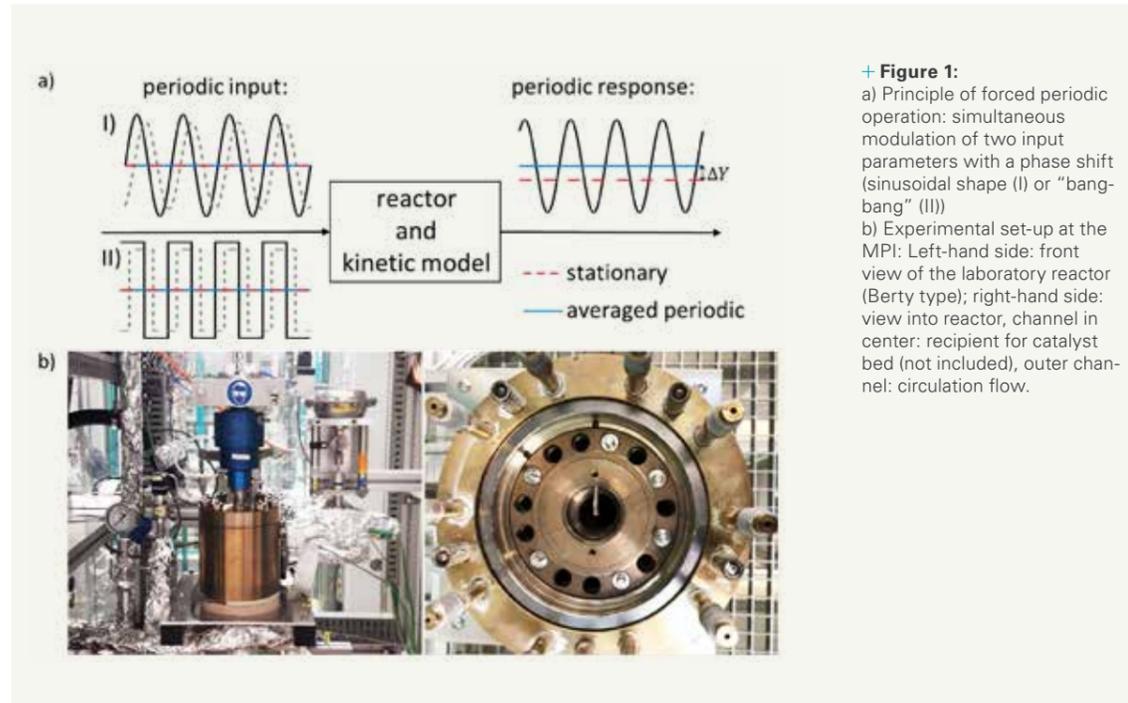


Author Dr.-Ing. Maria Gutierrez

Maria Gutierrez studied Chemical Engineering at the National University of Colombia. She received her Master's degree in Process, Energy and Environmental Systems Engineering from TU Berlin in 2014. In 2019, she obtained her Ph.D. at the National University of Colombia in the field of bioproducts process development. In 2021, she joined the PCF group as a postdoc and is focusing on process modelling and simulation.

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+ Figure 2:
 Schematic of the plant setup containing gas supply, laboratory stirred reactor and analytics (μ -gas chromatograph and mass spectrometer).

Forced Dynamic Operation of Methanol Synthesis

Larger quantities of chemicals are preferably produced in continuous operation by exploiting constant conditions at the reactor inlets. However, improved performance can be achieved by applying forced periodically varying inlet flowrates, inlet concentrations and/or inlet temperatures. The principle is illustrated in Fig. 1. Supported by the German Research Foundation (DFG) and in cooperation with the University of Belgrade (Serbia), the PSD and CSC groups at the MPI and the Faculty of Mathematics at Otto von Guericke University, theoretical concepts have been developed to identify optimal forced dynamic inlet parameters for any reaction system to increase time averaged product outlet streams compared to conventional steady state operation [1]. First successful experimental results were presented recently for a liquid phase hydrolysis reaction [2]. The subject of the current project is the experimental demonstration for an industrially relevant heterogeneous-catalyzed reaction, namely the synthesis of methanol synthesis.

The simplest aliphatic alcohol methanol (CH_3OH) is produced in large quantities. It is currently further increasing in importance. Due to the shift in the chemical industry and the transportation sector towards more sustainable processes, methanol is a potential fuel itself and an attractive hydrogen storage molecule. Being a liquid at ambient temperature, it is more suitable as an energy carrier than gaseous hydrogen.

Besides this, methanol is an important building block in the chemical industry for producing, for example, formaldehyde or acetic acid. As a reactant for methyl tertiary-butyl ether (MTBE) and dimethyl ether (DME), methanol is essential for synthesizing fuel additives and sustainable diesel substitutes.

Methanol is commonly produced at an elevated pressure of around 50 bar and temperature of 210–270°C from mixtures of CO_2 and syngas (CO and H_2) using solid catalysts. In order to produce the required syngas, fossil resources are currently exploited, which has a severe impact on the environment. In particular, the traditional production of hydrogen via methane reforming requires large amounts of energy and increases the carbon footprint.

Emissions from methanol production can be reduced or even fully avoided by substituting the fossil resources with renewable feedstocks. To achieve this goal, the production of energy and hydrogen can be altered by utilizing wind and solar based power. However, in connection with this transition, periodic fluctuations are unavoidable due to season, weather and time of day. Thus, varying inlet supplies will become a major characteristic of future chemical processes.

Our research project currently focusses on the experimental validation of predicted improvements of the methanol

synthesis by a forced periodic operation mode. A small-scale laboratory stirred steel reactor is used. The stirrer of this reactor generates a circulating gas flow through a bed of the catalyst ($\text{CuO}/\text{ZnO}/\text{Al}_2\text{O}_3$), on the surface of which the reaction takes place (see Fig. 1b). Due to the intense agitation gradient-less behavior is achieved, which supports the analysis of the experiments. In order to rely on an available model, that describes the kinetics of the reaction under dynamic conditions, the exclusion of intraparticle mass transfer phenomena is required [3]. The automated experimental set-up is equipped with gas composition measurements (μ -gas chromatography and mass spectrometry) and several mass flow controllers to implement the predicted component inlet flows (Fig. 2) [1, 4].

Currently, systematic testing of the equipment, including calibration of the mass flow controllers and analytics, is ongoing. Further investigations are devoted to characterizing the mixing behavior of the reactor and the residence time

distribution in the plant. After that, steady state experiments will serve as the benchmark, before the suggested forced periodic operation mode is tested in our isothermal well-mixed laboratory reactor.

Future activities will be devoted to studying non-isothermal tubular fixed bed reactors, since such reactors will be applied in possible large-scale industrial applications.

| Lothar Kaps, Wieland Kortuz

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Author Lothar Kaps

Lothar Kaps received his Bachelor's degree and his Master's degree in Chemical Process Engineering from Otto von Guericke University (OvGU) Magdeburg in 2019. During his Master's program, he studied at Niigata University, Japan, in 2017. After graduating with his Master's, he started his Ph.D. at OvGU in 2019. In 2022, he joined the PCF group at the MPI.

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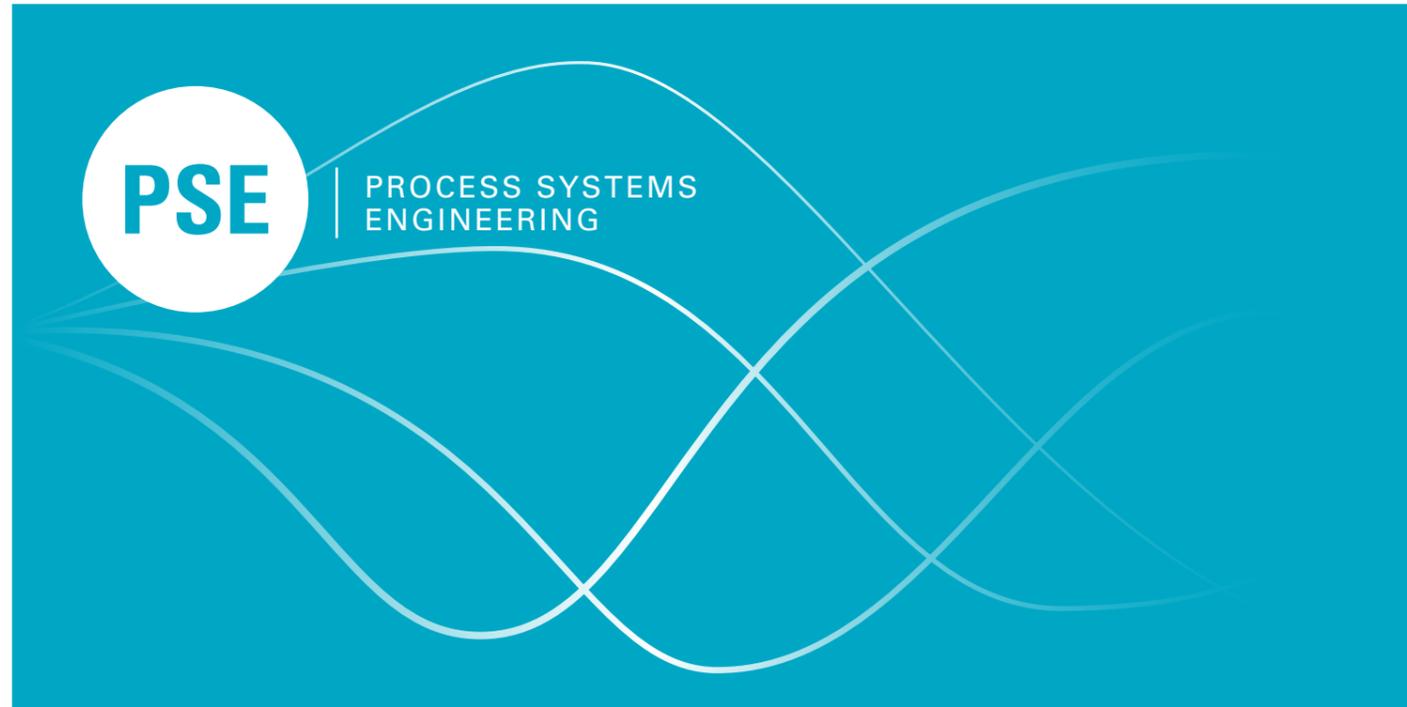


Author Wieland Kortuz

Wieland Kortuz studied Process Engineering and received his Bachelor's degree from the Anhalt University of Applied Sciences in 2019 and his Master's degree from Otto von Guericke University in Magdeburg in 2020. In the same year, he joined the PCF group as a Ph.D. student. His research focuses on the mechanistic description of reaction kinetics.

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+ Laura König-Mattern, Biosystems Engineer at the PSE group, is working up the lipid- and pigment-containing extract of the diatom *P. tricornutum* for HPLC-based pigment identification and quantification.

PROF. DR.-ING. KAI SUNDMACHER | DIRECTOR

In recent decades, we have seen continuous progress in increasing the productivity and selectivity of (bio-) chemical and energy conversion processes. Nevertheless, to cope with the great challenges of the future, new breakthroughs in **Process Systems Engineering** are necessary in order to achieve drastic performance improvements in existing processes, to invent dream process technologies for synthesizing chemicals and transforming energy at the highest level of resource efficiency, to strongly accelerate the transition from fossil to renewable raw materials, to organize a comprehensive circular economy for as many material streams as possible, and - at the same time - to achieve even higher product quality and functionality objectives.

This vision statement forms the background to the PSE group's research mission. We closely combine **mathematical modeling** of complex process systems with theoretical methods for **process analysis, synthesis, and optimization** as well as with **experimental validation** techniques. Over the last few years, we have developed the elementary process functions (EPF) methodology that supports process design decisions at multiple levels of the process hierarchy

(molecular level, phase level, process unit level, plant level). Recently, we have extended this EPF methodology to complex process networks (FluxMax approach) and applied the same to derive methanol production systems that are only fed with renewables.

In the **Chemical Production Systems** research field, our focus was on multiphasic reaction and liquid-liquid extraction processes using thermomorphic multicomponent mixtures, ionic liquids, and deep eutectic solvents. This research was carried out partly in cooperation with TU Berlin, TU Dortmund, and Otto von Guericke University under the umbrella of the DFG-funded Collaborative Research Center "InPROMPT". Regarding the computer-aided molecular design of solvents and adsorbents, we have continued to collaborate with the group led by Prof. Zhiwen Qi at ECUST in Shanghai. Moreover, we have started a new research project on plastics recycling (MaxDePoly) to identify energy-saving solvolytic pathways for decomposing polyamides into their monomers. We are very grateful that the Supporting Members of the Max Planck Society sponsored this project with generous donations.

Regarding **Energy Conversion Systems**, we have investigated novel Power-to-X processes for the efficient conversion of electrical energy into hydrogen, methane, methanol,

Fischer-Tropsch hydrocarbons, and ammonia. These activities are directly linked to the BMBF flagship project "H₂Mare/Power-to-X Wind", in which our PSE group is involved together with more than 20 other partners. Due to the volatility of renewable energies, the flexible and safe operation of catalytic reactors is becoming increasingly important. To this end, we have derived a core-shell catalyst design for CO₂ methanation using mathematical optimization and confirmed its functionality with experiments (see pages 42-43). This work was done under the umbrella of the DFG priority program "Catalysts and Reactors Under Dynamic Conditions for Energy Storage and Conversion".

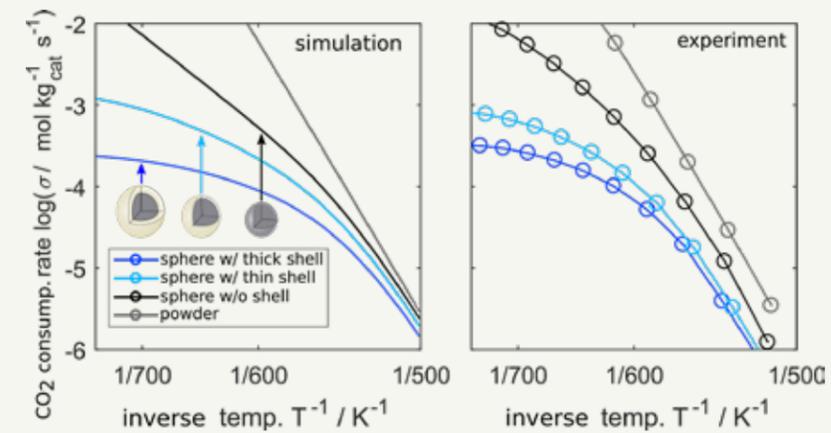
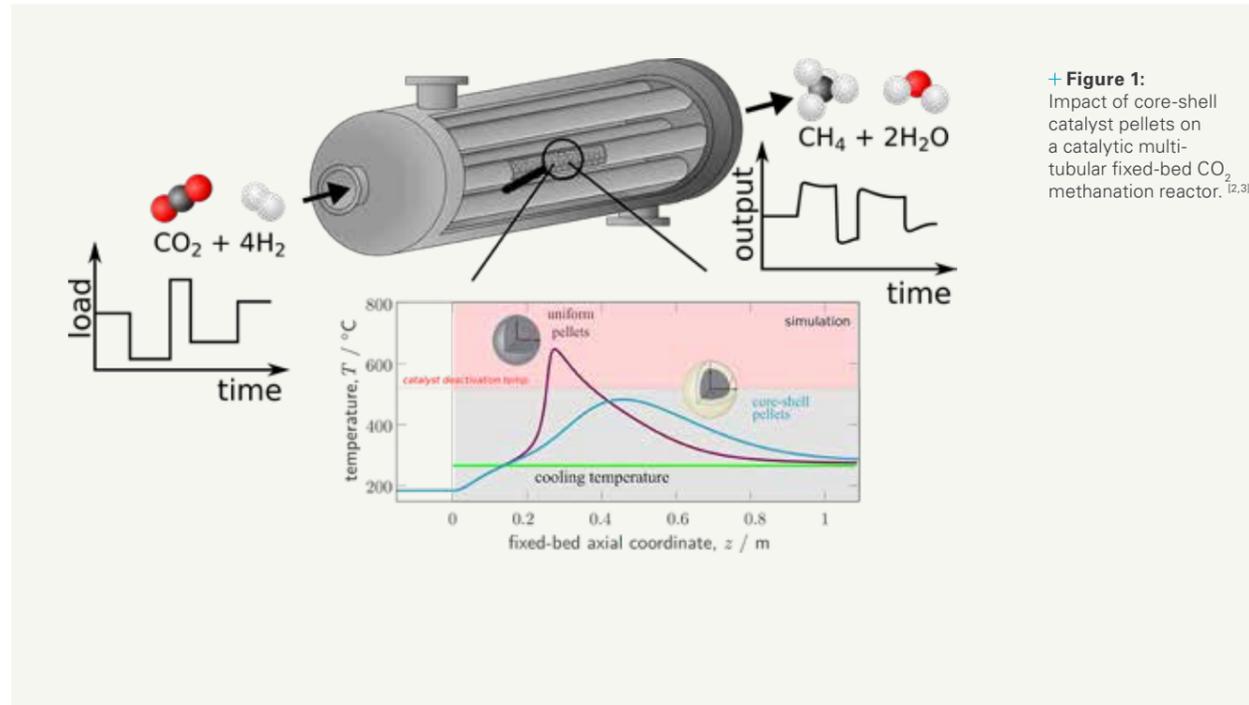
In the field of **Biological Production Systems**, we focused our research efforts on the computer-aided design of a green microalgae biorefinery using *Phaeodactylum tricornutum* as a model organism. We found that, by solvent-based fractionation of wet algal biomass into carbohydrates, proteins, lipids, and pigments, there is no need for an energy-intensive biomass drying step. Via computational screening in large databases, we identified 2-butanol as a highly effective, green solvent that outperforms the toxic benchmark solvent n-hexane (see pages 44-45). Moreover, we continued our research on synthetic biosystems, aiming at the systems-oriented modular assembly of artificial cells from biomolecular functional units. In this project, we gained a deep under-

standing of the charge-mediated fusion phenomena of cell-like vesicular compartments built from polymer/lipid hybrid membranes. Special experiments to track vesicle fusion events were carried out in collaboration with the MPI for Colloids & Interfaces in Potsdam and Martin Luther University in Halle.

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Load-Flexible Reactors and Core-Shell Catalysts for Power-to-X Processes

The European Council has endorsed the goal of making the European Union carbon-neutral by 2050. To achieve the required reduction in carbon dioxide emissions, a massive expansion of electricity generation from renewable sources is required, which will ultimately drive the demand for novel power-to-X processes. In this context, surplus renewable energy is used for hydrogen production by electrochemical water splitting. Subsequently, hydrogen is converted into easily distributable chemical energy carriers such as methane, methanol, or ammonia. In particular, the synthesis of carbon-based products offers the opportunity for reducing carbon dioxide emissions by consuming CO_2 as a reactant.

Catalytic multi-tubular fixed-bed reactors are a key technology for large-scale, low cost chemical synthesis. However, changing market conditions and fluctuating process inputs (e.g., due to volatile renewable energy supply) currently require reactor and catalyst designs that work well not only at a fixed nominal load point, but also at varying partial loads. During dynamic scenarios, it is often unclear how load transitions should be performed, how much time the load transition requires, and whether there is a risk of material damage. From our theoretical considerations, we have already been able to derive several, often non-intuitive phenomena, which have been confirmed experimentally [1]. In particular, the occurrence of so-called thermal runaways makes load-flexible operation of such reactors a challenging task. In this context, our research activities

are focused on simulating and optimizing fixed-bed reactors by combining computational and experimental approaches.

On the computational side, the core of our research work is a multi-scale fixed-bed reactor model. This model considers an industrial-scale multi-tubular reactor surrounded by a cooling jacket. The model includes heat and mass transfer correlations as well as a detailed catalyst pellet model. All model components are solved numerically as a large differential-algebraic system of equations, to simulate a variety of technical scenarios (e.g., startup, shutdown, load-changes). In addition to simulation, rigorous optimization studies are employed to identify promising, novel catalyst design concepts. In process systems engineering, such profound in-silico analyses are essential for building sound knowledge and formulating scientific hypotheses that justify cost-intensive technical implementations.

In our simulation studies, various reactor concepts (e.g., intensified reactors, recycle reactors) were analyzed within the expected operating range. Thereby, feasible operating points are declared as points featuring sufficient carbon dioxide conversion at the reactor outlet (e.g., $X_{\text{CO}_2} > 95\%$) and a maximum reactor temperature below the catalyst deactivation temperature (e.g., $< 500^\circ\text{C}$). We found that core-shell catalyst pellets, consisting of a catalytically active core surrounded by an inactive but porous shell, are beneficial in this regard. The advantages compared to uniformly active catalyst pellets

include a significantly decreased maximum reactor temperature (as seen in Figure 1), an increased methane yield, and a faster response behavior to load changes. In this way, an economic, safe, and load-flexible fixed-bed reactor operation at industrial scale is possible. [2]

A detailed comparison to the well-established fixed-bed dilution with inert catalyst pellets has shown that the benefits of the core-shell catalyst concept arise from the mitigation of the reaction rate by the inert shell, in particular at high reactor temperatures. Hence, the inert shell prevents significant temperature excursions, which could damage catalyst and reactor material, while allowing for high CO_2 conversions at the same time. Systematic sensitivity studies regarding relevant reactor design and operating parameters showed that a robust technical implementation of these catalyst pellets is possible by coating commercially available uniform catalyst pellets with an inert layer [2, 3].

Inspired by the theoretical results, we coated uniform catalyst pellets with an inert layer in a fluidized-bed coating plant at pilot-plant scale. Based on detailed morphological and catalytic analyses, the experimental results are in line with the computationally predicted trends, as shown in Figure 2. In particular, the core-shell catalyst pellets exhibit the expected Arrhenius-law temperature dependency at low temperatures and an approximately constant reaction rate at high temperatures, which is necessary for the formerly discussed advantages to be present [4]. In further experiments, the catalyst pellets will be investigated in more detail in a so-called “single-pellet-string reactor”, which allows for the derivation of a detailed reaction kinetic model.

In summary, our findings underline the importance of combining computational and experimental approaches

for designing innovative processes that convert renewable energy into valuable, easily distributable chemical energy carriers. Future work will focus primarily on the extension and validation of our novel catalyst concept to other reaction systems of industrial importance. | Ronny Tobias Zimmermann

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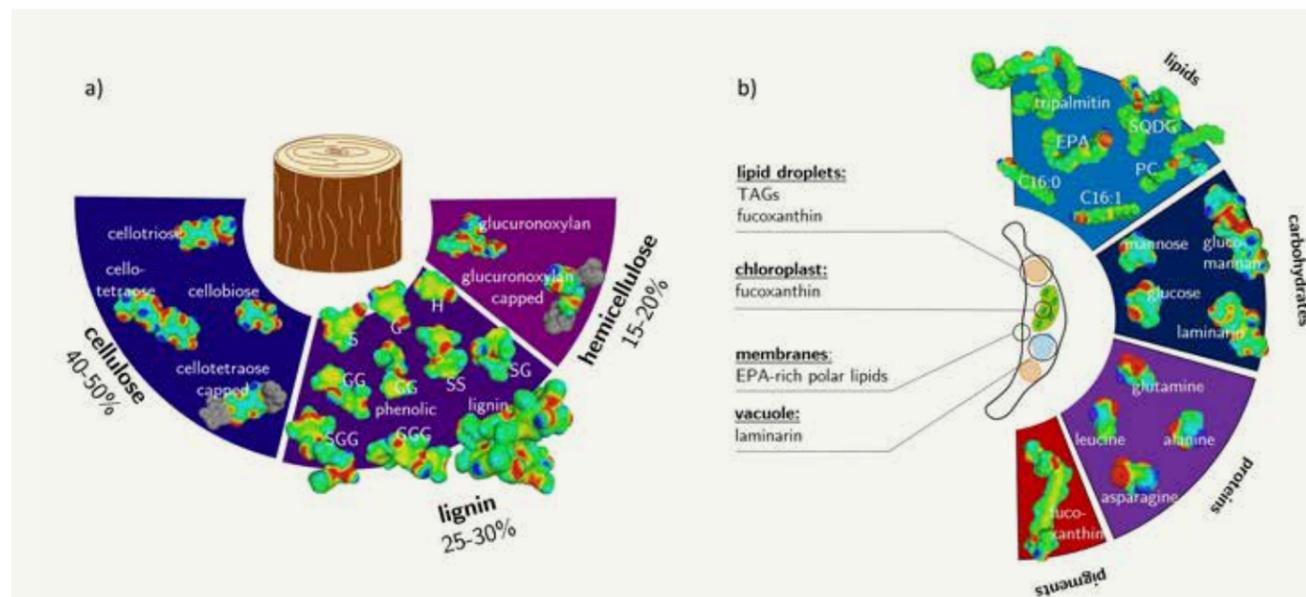
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Author Ronny Tobias Zimmermann

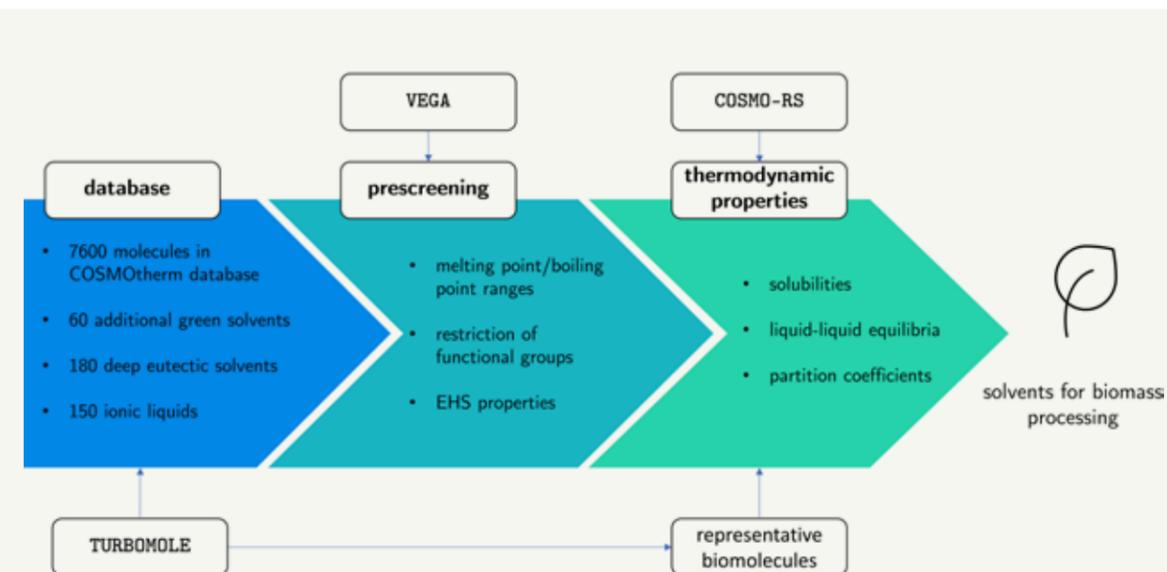
Ronny Tobias Zimmermann embarked upon his academic career in 2012 with his Bachelor's studies in Chemical and Biological Engineering at FAU Erlangen-Nuremberg. During this time, he worked as an intern at a local biogas plant and at Evonik Industries AG, where he modelled and simulated a polymer production plant. He received his Master's degree from FAU Erlangen-Nuremberg in 2018 after completing his thesis in Professor Freund's Research Group. Since May 2018, he has been working in the PSE group headed by Professor Sundmacher, focusing on the impact of catalyst pellet design on the operation of fixed-bed reactors for Power-to-Gas applications.

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+ **Figure 1:**
Approach for the computational solvent screening framework.



+ **Figure 2:**
Representative biomolecules for each biomass fraction of a) lignocellulosic biomass and b) algal biomass.

Computer-Aided Solvent Selection for Biomass Processing

Depleting fossil resources and ongoing climate change are global challenges of this century. While a growing human population must be provided with adequate food and energy, climate-damaging greenhouse gases also need to be reduced drastically. Therefore, a transformation of current fossil-based processes into sustainable production routes based on renewable energy and bio-based raw materials is required. In this light, biorefineries have emerged as resource-efficient concepts aiming at a waste-free use of biomass. In a “zero-waste” biorefinery, the biomass feedstock is fractionated into its main macromolecular constituents, which subsequently serve as building blocks for the sustainable production of chemicals, for the manufacturing of bio-based materials or for energetic use.

In a biorefinery process, solvents are commonly applied to assist biomass fractionation. The solvent choice is an important decision for the overall process as it determines the efficiency of the extraction, the purity of the products, and the sustainability and economic viability. However, the solvent choice is highly dependent on the type of biomass to be processed and the required process conditions.

In order to facilitate systematic and rational solvent selection for the processing of various feedstocks, we developed a computational solvent screening methodology. We screened a database of more than 8000 potential solvents for two

types of biomass: lignocellulose and microalgae. For each type of biomass, the database was screened for solvents with suitable melting and boiling points as a first step. As the solvents being used in a biorefinery should be non-hazardous, we used quantitative structure-activity models to predict environmental, health and safety (EHS) criteria of the potential solvents. Furthermore, we modelled representative biomolecules using quantum chemical calculations in order to mimic each fraction contained in the biomass. These representative biomolecules were subsequently used for COSMO-RS solubility predictions in the solvent candidates. As the biomass fractions need to be separated from each other, we predicted the phase behavior of biphasic solvent mixtures and partition coefficients of the biomolecules. This framework enables the selection of the most promising solvent candidates in terms of solubility and EHS criteria.

We applied the screening framework to lignocellulose, as this type of biomass is the most abundant source of biomass-bound carbon^[1]. Lignocellulosic biomass contains cellulose, hemicellulose and lignin as the three major components. While the cellulose and hemicellulose sugars serve as building blocks for fuel and chemical production, lignin is one of the few renewable sources for the production of aromatics. Lignocellulosic biomass is recalcitrant to mechanical and chemical attack, requiring harsh process conditions. To date, solvents applied in lignocellulose processing suffer

either from high toxicity, such as 1,4-dioxane, or from low lignin solubility, such as alcohols. We therefore applied the developed solvent screening framework to identify solvents with high lignin solubility and benign EHS properties. We identified several sulfoxides, azines, phosphonates, oxazolines, and cyclic ethers to be very promising candidates for the typical “lignin first”-approach. Solubility measurements of different types of lignin in the identified solvents showed high lignin solubilities of more than 33 wt.% and beneficial EHS-related properties.

Another promising source of biomass is green microalgae. Due to their high growth rates, cultivation on non-arable land and the production of high-value molecules, microalgae have received much interest in recent years. After harvest, the moisture content remains at ca. 85 wt.%. Usually, the algal biomass is under high energy consumption before the valuable molecules are extracted with the cheap but toxic solvent n-hexane. Several studies have shown that the drying step renders the overall process economically infeasible. However, n-hexane is hydrophobic and can hardly penetrate the wet algal cells. Therefore, we applied our novel screening framework to identify solvents for the extraction of carbohydrates, proteins, lipids and pigments from wet microalgae^[2]. We identified 2-butanol as an interesting solvent candidate. 2-butanol is partially water-miscible and therefore miscible with the moisture contained in the algal cells, allowing access to the valuable algal molecules. After adding additional water beyond the miscibility limit, two liquid phases are formed. In the biphasic system, carbohydrates and proteins are separated from lipids and pigments. The yield of lipids and pigments after 2-butanol extraction is significantly higher compared to the traditionally used solvent n-hexane. 2-butanol achieves similar high lipid and pigment yields as ethanol. However, in contrast to ethanol, 2-butanol

has the advantage of forming a biphasic system with water, which allows for an integrated fractionation step.

Currently, we are expanding our work to machine learning-based solvent design which sheds light on so-far unexplored classes of solvents with high potential for application in biorefinery processes. | **Laura König-Mattern**

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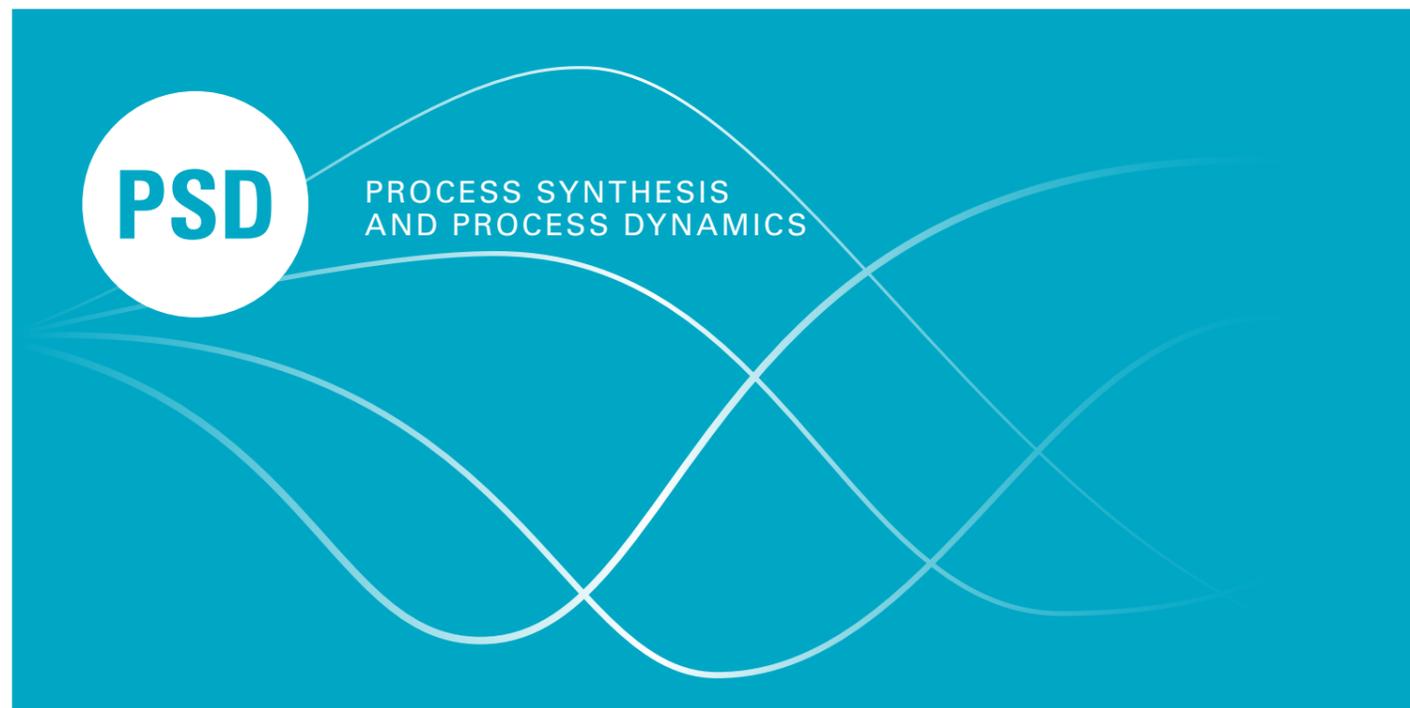
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Author **Laura König-Mattern**

Laura König-Mattern studied Biosystems Engineering at Otto von Guericke University in Magdeburg from 2013 to 2017, where she was intrigued by the mathematical modeling of (bio)chemical processes and coding. To deepen her knowledge in this field, she studied Systems Engineering and Engineering Cybernetics in Magdeburg and graduated with a master's degree in 2019. She then started her Ph.D. in the PSE group headed by Prof. Sundmacher, where she has since been working on a systematic method for solvent screening and design in the field of biomass processing. In 2021, she was awarded a fellowship from the Christiane Nüsslein-Volhard Foundation and received a science communication award from the BMBF. Since October 2022, she has been a visiting Ph.D. student in the group of Prof. Luterbacher at École Polytechnique Fédérale de Lausanne.

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+ Stefanie Duvigneau is preparing the parallel bioreactor system for a new experimental setup, while Annette Wilisch-Neumann and Achim Kienle are discussing recent results of the Fourier-Transformations-Infrared-(FTIR) Spectroscopy.

PROF. DR.-ING. ACHIM KIENLE |
EXTERNAL SCIENTIFIC MEMBER

+ The Process Synthesis and Dynamics (PSD) group is headed by Achim Kienle, who is an external scientific member of the MPI. He also holds a professorial position at Otto von Guericke University. His MPI and university groups collaborate closely.

The PSD group develops methods and tools for the synthesis, analysis, and control of complex process systems. It combines physical chemical insight with concepts from systems and control theory as well as applied mathematics. Process insight guides the way to suitable problem formulations and to feasible, efficient solution strategies. Whenever possible, theoretical concepts are validated experimentally. With its approach, the PSD group helps to bridge the gap between theory and application.

Process control has emerged as a major field of research for the PSD group during the last decade. Currently, the focus is on the control of particulate processes, advanced chromatographic processes, and methanol synthesis, which is an example of a particular important and challenging reaction

system. Particulate processes are described by nonlinear partial differential equations and represent a highly challenging class of distributed parameter systems. Important topics addressed by the PSD group include mathematical modeling, nonlinear model reduction, and new approaches to robust and nonlinear control of particulate processes. Novel crystallization, fluidized bed spray granulation, and agglomeration processes have been investigated as interesting application examples. Chromatographic processes are switched systems with cyclic behavior. A particular focus of the PSD group has been online parameter estimation, optimization, and adaptive cycle-to-cycle control of simulated moving bed chromatographic processes, which play an important role in difficult separation problems in fine chemistry, including the pharmaceutical industry. Novel challenges for the control of methanol synthesis are posed by new applications for chemical energy storage under randomly fluctuating conditions. Furthermore, new modes of forced periodic operation are being developed together with the Seidel-Morgenstern group from the MPI and the Petkovska group from Belgrade University.

In the field of **Process design**, the PSD group is developing computational methods for a systematic design of complex process systems. Approaches range from shortcut methods

based on analytical insight up to rigorous simultaneous mixed integer nonlinear optimization (MINLP) of process configurations, operating conditions, and auxiliary materials. During the period covered by this report, particular emphasis was placed on new methods for integrated molecular and process design for liquid multiphase reaction systems using hierarchical MINLP optimization approaches and on novel analytical and numerical methods for chromatographic processes with finite mass transfer resistance and/or axial dispersion.

Biosystems engineering has been identified as a research area of common interest at the Max Planck Institute and the Otto von Guericke University. The PSD group makes important contributions to biosystems engineering in the fields of modeling, nonlinear dynamics, and control of biotechnological processes. Special emphasis during the period covered by this report was on multiscale modeling to describe cell-to-cell heterogeneity in vaccine production processes and polymer properties in microbial biopolymer production processes. Furthermore, the group has contributed to the institute's activities in the innovative field of conceptual modeling and analysis of synthetic biological systems.

The PSD group has been involved in a number of highly visible larger joint research projects with external funding,

including the joint research center Transregio SFB 63 on integrated chemical processes in liquid multi-phase systems. This involves around 15 other partners, mainly from TU Berlin and TU Dortmund. Furthermore, the group is participating in several nationwide priority programs with funding from the German Research Foundation (DFG), including SPP 2080 on catalysts and reactors under dynamic operating conditions for energy storage and transformation, SPP 2331 on machine learning in chemical engineering, and SPP 2364 on autonomous processes in particle technology.

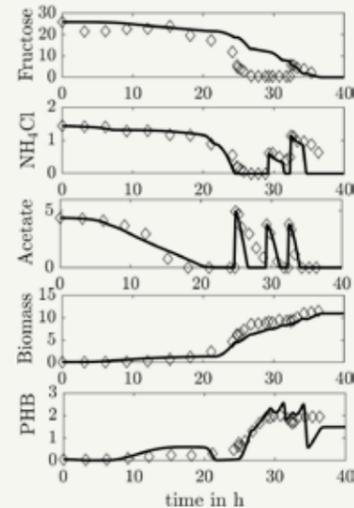
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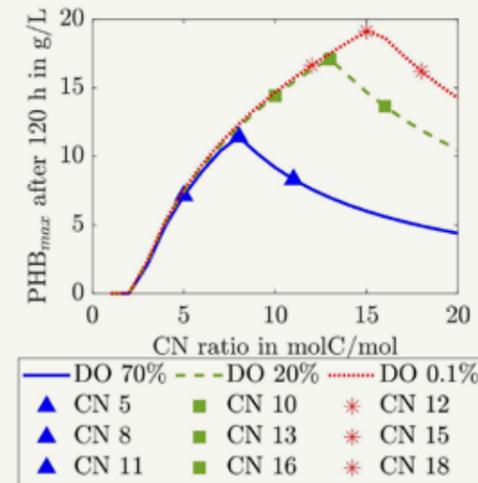




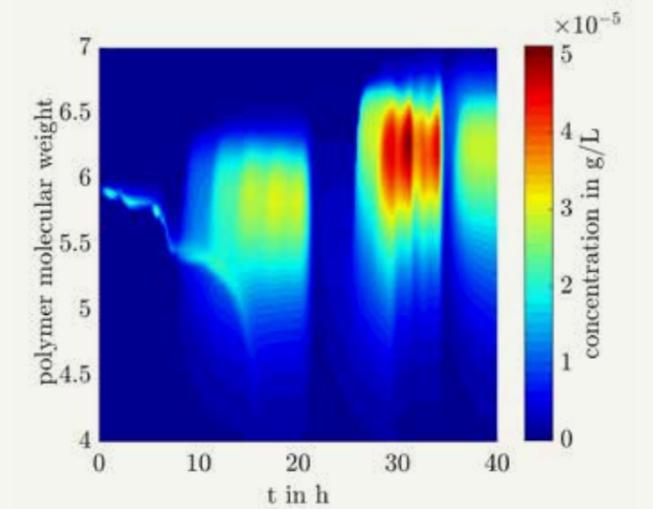
+ **Figure 1:**
Sampling procedure on a small-scale bioreactor.



+ **Figure 2:**
Dynamic behavior of substrate and product concentrations in [g/l] during PHB production with fructose and sodium acetate as carbon sources [2].



+ **Figure 3:**
Simulation study to investigate different carbon-to-ammonium (CN) ratios and dissolved oxygen (DO) levels on PHB polymer yields [2].



+ **Figure 4:**
Dynamic behavior of PHB polymer weight distribution in log10 [g/mol] corresponding to Fig. 2 [3].

Tailor-Made PHA Biopolymers From Waste

+ Polyhydroxyalkanoates (PHAs) are an interesting class of biopolymers. They are produced by many microorganisms under unbalanced growth conditions (e.g., lack of nitrogen or phosphate) for intracellular storage of carbon and energy. In contrast to conventional petroleum-based polymers, PHAs are biologically degradable under ambient conditions and could contribute significantly towards reducing environmental pollution caused by plastic waste. PHAs can be produced sustainably from renewable resources, carbon dioxide, or biogenic wastes and residues. Depending on the microorganism and the substrates, polymers with different properties are formed. Polymer properties mainly depend on polymer composition and its molecular weight distribution.

Despite these advantages, the market share of PHAs is still relatively low. To increase this share, production costs need to be reduced. In our research, we aim to reduce costs by using waste streams from food industries as cheap substrates and applying model-based control to increase the polymer yield and adjust the polymer properties to the desired specifications. For this purpose, we developed a multiscale modeling approach and applied it to example processes with carbon sources often occurring in waste streams from food industries. Our approach couples metabolic models with polymerization kinetics to predict PHA yields and properties depending on the cultivation conditions.

An example of the results predicted by the metabolic modeling is shown in Fig. 2 for the microorganism *Cupriavidus necator* using a mixture of fructose and acetate as carbon sources leading to the production of polyhydroxybutyrate (PHB). Following the ideas in [1], the model assumes optimal intracellular regulation of the microorganism in view of available resources as a consequence of evolution. Thereby, it allows a relatively simple and elegant approach to predict dynamic behavior. In addition, the influence of dissolved oxygen in the medium on metabolism was considered, as described in [2]. Theoretical predictions are in good agreement with experimental data obtained in our lab, as shown in Fig. 2.

The metabolic model can be used to predict and optimize the effect of cultivation conditions on polymer yields, as illustrated in Fig. 3. The relevant parameters in this diagram are the carbon-to-ammonium ratio (CN) and the dissolved oxygen (DO) level. The results show that smaller DO levels facilitate higher final PHB yield because more carbon can be transferred to PHB production.

The temporal evolution of the molecular weight distribution for the setup shown in Fig. 2 can be predicted by our multiscale model and is shown in Fig. 4 [3]. It can be used to predict not only polymer yields but also polymer properties at the end of the batch, depending on the cultivation conditions. Conversely,

the model could be inverted to calculate the optimal cultivation conditions to achieve the desired polymer properties. A direct inversion is mathematically challenging. Therefore further research is being carried out in our group to replace such a direct inversion by recursive algorithms using feedback control.

If propionic acid is used as a second substrate instead of acetate, the co-polymer PHBV is synthesized instead of the homo-polymer PHB [4, 5]. PHBV is more flexible than PHB and, therefore, easier to handle for further processing. However, propionic acid is limiting biomass growth significantly. The multiscale modeling approach has been used to find an optimal compromise between the two conflicting goals. Future research will also focus on more advanced PHAs to open new fields of application for this interesting class of biopolymers.

! **Stefanie Duvigneau, Robert Dürr**

Author **Stefanie Duvigneau**

Stephanie Duvigneau studied 'Biosystems Engineering' at Otto von Guericke University Magdeburg and received her master's degree in 2015. She then joined the PSD group and became a member of the International Max Planck Research School ProEng. She has worked on multiscale modeling of influenza vaccine and PHA biopolymer production processes and defended her Ph.D. thesis in spring 2023.

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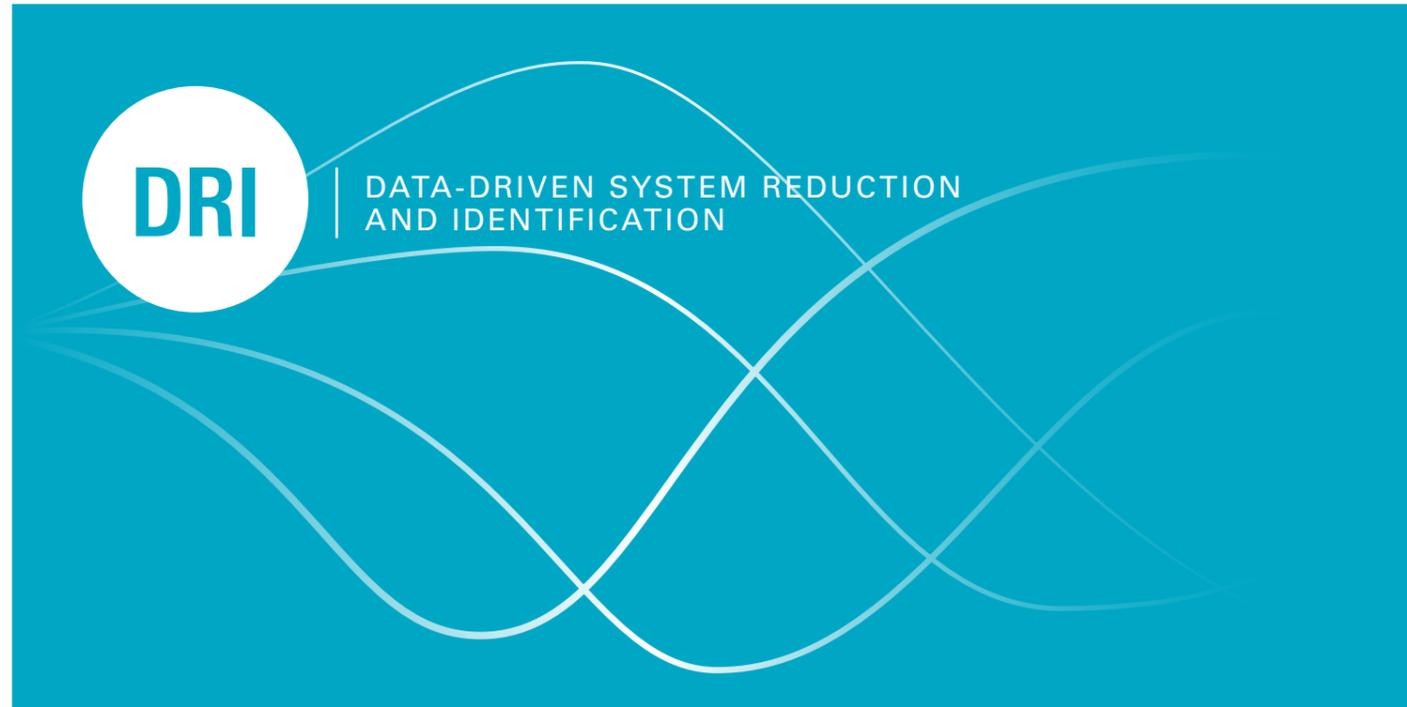
Robert Dürr studied 'Systems Engineering and Engineering Cybernetics' at Otto von Guericke University Magdeburg and received his diploma in 2009. Afterwards, he joined the PSD group where he worked on population balance modeling and simulation of vaccine production processes. After finishing his Ph.D. with honors in 2016, he was a postdoctoral fellow at the Department of Chemical Engineering at KU Leuven (Belgium) and at the PSD group. Since 2021, he has been Professor for Engineering Mathematics at Magdeburg-Stendal University of Applied Sciences. His recent fields of research comprise multiscale modeling and control of microbial biopolymer production, as well as particle formation processes.

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www.mpi-magdeburg.mpg.de/psd



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+ Figure 1: The DRI group, Toepffer-Villa, Magdeburg, July 2022.

PROF. DR. ATHANASIOS C. ANTOULAS |
MAX PLANCK FELLOW

The data-driven system reduction and identification (DRI) group has been led by Professor Antoulas since 2017 (Fig. 1, centre). In addition, the DRI group consists of one postdoctoral researcher, Dr. Ion Victor Gosea (Fig. 1, left), and one doctoral student, Dipl. Eng. Dimitrios Karachalios, M.Sc. (Fig. 1, right).

The DRI group carries out mathematical research with the main focus on studying classical tools on numerical linear algebra and system theory, together with the development of methods in reduced-order modeling, learning dynamical models from measurements and model reduction from a data-driven perspective.

In recent years, one of the main challenges has been to correctly quantify and interpret the information that can be extracted from data measurements. In many engineering disciplines (e.g., electrical, mechanical, or electro-chemical engineering) the typical way of providing solutions is by means of linearizing complex nonlinear systems. This approach has its own limitations since linear approximations to nonlinear problems are only locally successful.

Moreover, the derived theoretical models may also have missing terms which cannot explain the data under noisy conditions. In the modeling stage, when more features are included, this inevitably leads to the “curse of dimensionality”. Therefore, one successful way of overcoming such problems

is to introduce model order reduction. Classical methods such as balanced truncation have made model reduction techniques popular and reliable by providing error bounds. These methods are difficult to apply when only input-output data are known, the system’s quantities (matrices) are not explicitly known or the model is too complicated to be dealt with.

In recent years, *machine learning* (ML) techniques have aimed at learning the dynamics associated with the “black box” hidden model. By combining learning procedures from data, alongside complexity reduction techniques, it is desired to devise approaches that yield reduced models from data (toward the discovery of dynamical systems). A classical way to implement model reduction methods is by employing interpolation. One method under consideration, known as the *Loewner framework* (LF), is a non-intrusive interpolatory model order reduction technique that can achieve identification of the black box systems when solely data measurements are available (input-output data, either in the time or in the frequency domain). LF can also be viewed as a data-driven interpolation-based identification and reduction approach that uses measured or computed data to construct surrogate models of low complexity. It has been continuously developed and applied to various problems over recent decades. The activity of the DRI group has been mostly (although not entirely) focused on advancing and extending this framework to different applications; in particular, we mention the L-DDC (Loewner Data-Driven Control) approach, originally developed at Onera, France, and the application of LF to the diagnosis of faulty behavior in electrochemical systems (such as fuel cells), here at the MPI (advanced through the Ph.D. program of Mr. Patel). Additionally, the

extension of LF to the learning of reduced-order nonlinear models (from time-domain data) was advanced significantly through the Ph.D. program of Mr. Karachalios (2017{2022).

Internal and external scientific collaboration

The following are internal collaborations within the MPI Magdeburg:

1. Joint work with the CSC group led by Prof. Peter Benner (also collaborating with Dr. Igor Pontes Duff, Jun. Prof. Jan Heiland, Dr. Quirin Aumann, Prof. Alexander Zuyev, Kirandeep Kour, and Leonidas Gkmissis) on model reduction of infinite-dimensional linear systems, of linear systems with differential algebraic terms, hybrid moment matching approaches for multi-input multi-output systems, reduction of linear switched systems.
2. Joint work with the EEC group led by Dr.-Ing. Tanja Vidaković-Koch (including Dr. Antonio Sorrentino and Dr. Luka Zivković); the scope was applying the Loewner framework for the frequency response analysis of fuel cells (linear and nonlinear analysis).

The following are external collaborations outside of the MPI Magdeburg:

1. Joint work with Prof. Matthias Heinkenschloss (Dep. of Applied Mathematics, Rice Univ., Houston, TX, USA) on various model reduction topics (including model reduction of quadratic systems with quadratic outputs).
2. Joint work with Dr. Mihaly Petreczky (Lille, France), Dr. John Leth, and Prof. Rafael Wisniewski (Aalborg, Denmark) on modeling switched and hybrid systems.

3. Joint work with Prof. Serkan Gugercin and Prof. Christopher Beattie (Virginia Tech, Blacksburg, VA, USA) on various data-driven modeling techniques.

4. Joint work with Dr. habil. Charles Poussot-Vassal (Toulouse, France) on data-driven control and infinite-dimensional model reduction (additionally, an invited research visit was undertaken by Dr. Ion Victor Gosea to the Onera Institute, September 13{17, 2021).

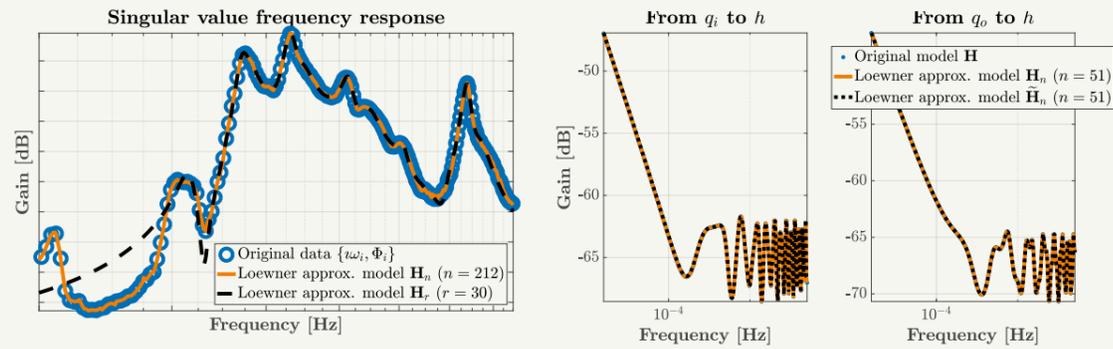
5. Joint work with Dr. Benjamin Unger (Stuttgart, Germany) on parametric model reduction (additionally, an invited research visit was undertaken by Dr. Ion Victor Gosea to the Simtech Institute, University of Stuttgart, September 20–24, 2021).

6. Joint work with Dr. Steffen Werner (Courant Institute, New York, USA) on data-driven model reduction of mechanical systems.

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+ Figure 1: Loewner fit on the data (left) & approximation by the Loewner rational function (right).

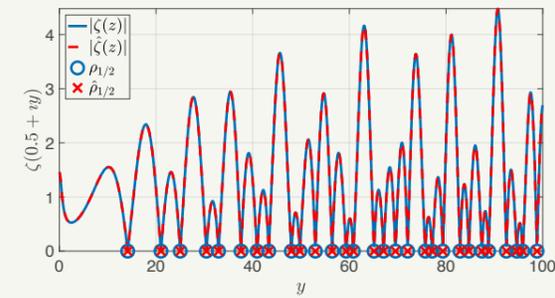
Data-Driven Reduced-Order Modeling and Control

+ **Introduction** The Loewner Framework (LF) was initially introduced to provide elegant, direct solutions to the identification and complexity reduction problems through the lens of rational approximation. LF is a data-driven method that requires frequency response data and does not require a complex optimization step. An application of LF that has been adopted fairly recently is specifically for the purpose of data-driven control; LF can be used as a tool for feedback controller design as in traditional loop shaping methods, to fit a reference controller in terms of **input-output data** and not by means of a model, i.e., in the traditional way.

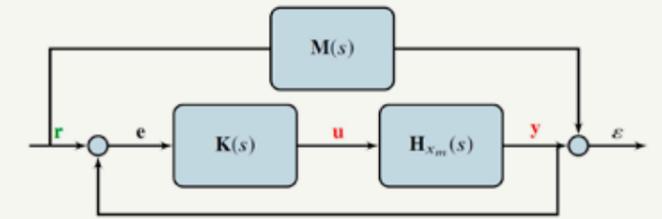
LF as a data-driven reduced order modeling tool The data set typically contains samples of the transfer function (TF). These can be measured or computed by direct numerical simulations. The setup in [1] is as follows: vibration problems are often detected in aircraft engineering (causing fatigue and comfort issues). Anti-vibration controllers need to be designed using a model, targeting undesirable amplifications of the aerodynamical effects on the fuselage around some specified frequencies. However, reliable and simplified models are seldom available. Ground Vibration Tests (GVTs) are performed to validate both the control performances and the original model. The benchmark in [1] illustrates generic GVTs, performed on a particular aircraft model for which robust control laws need to be implemented. Using shakers applied at some locations, the structure is excited, thus simulating

aerodynamic disturbances. The LF is able to accurately recover the transfer function from data, as observed in the left part of Fig. 1. It allows readjustment of the theoretical models with upcoming experiments, to detect new phenomena and re-tune the control laws. This step contributes to the quest of constructing a reliable **digital twin** infrastructure.

Approximation of infinite-dimensional linear systems Rational functions can approximate well functions with singularities and with oscillatory behavior better than polynomials can. Furthermore, rational functions are extensively used in systems and control theory since the input-output behavior of linear dynamical systems is described in the frequency domain by the so-called transfer function (which is indeed a rational function). Recently, in [5], LF was applied for approximating non-rational transfer functions, which characterize the input-output behavior of infinite-dimensional linear systems. We mention here the Bessel function and also an Euler-Bernoulli vibrating beam model. Additionally, in [3], a data-driven analysis of transfer functions corresponding to the Saint-Venant (or shallow water) equations was presented. These are largely used in hydraulics to model the dynamics of an open channel flow. These equations consist of two nonlinear hyperbolic PDEs. In the considered test case [3], under mild simplifying assumptions detailed there, a particular setup is constructed. The LF approach was shown to provide a good approximation quality (see the right part of Fig. 1); a post-processing tool



+ Figure 2: Matching of the ζ function zeros (left) & data-driven control problem formulation (right).



that enforces the asymptotic stability of the ROMs was also applied in [3]. Finally, in [4], the Loewner matrix pencil is used to identify the non-trivial harmonic zeros of ζ , the Riemann zeta function. The application targeted here is the accurate approximation of the prime counting function. As depicted in the left part of Fig. 2, the method correctly identifies all the zeros of the irrational function in a particular interval (here, inside $[0; 100]$), hence detecting how many prime numbers appear in that particular range.

Frequency-domain DDC (standard) rationale The DDC approach discussed in [1, 2] is based on the 2002 contribution of Campi et al., which was recently extended to the frequency-domain, in the works of Kergus, Vuillemin, and Pousot-Vassal. As depicted in the right part of Fig. 2, the system to be controlled is described by H . This latter is considered unknown while frequency-domain input-output data are accessible. Then, M is the so-called objective closed-loop transfer function. This latter defines the expected response to be imposed on the system when the controller is inserted in the looped architecture. The objective is to find a controller K minimizing the difference between the resulting closed-loop and the reference model M . This is made possible through the so-called ideal controller K^* : the LTI controller that would give the desired reference model frequency-domain behavior if inserted in the closed-loop. Finding a controller K that fits the data can be considered to be an identification problem. In [2], this latter is considered through the lens of both data-driven interpolatory, and least-squares methods. This is done by comparing the methods LF, the AAA Algorithm, and vector fitting (VF). More involved results are shown in [1]. There, it was shown that through the L-DDC procedure, one can compute reduced-order controllers which faithfully mimic the ones constructed through model-based approaches, such as proportional integrator (PI) controllers. **Ion Victor Gosea**

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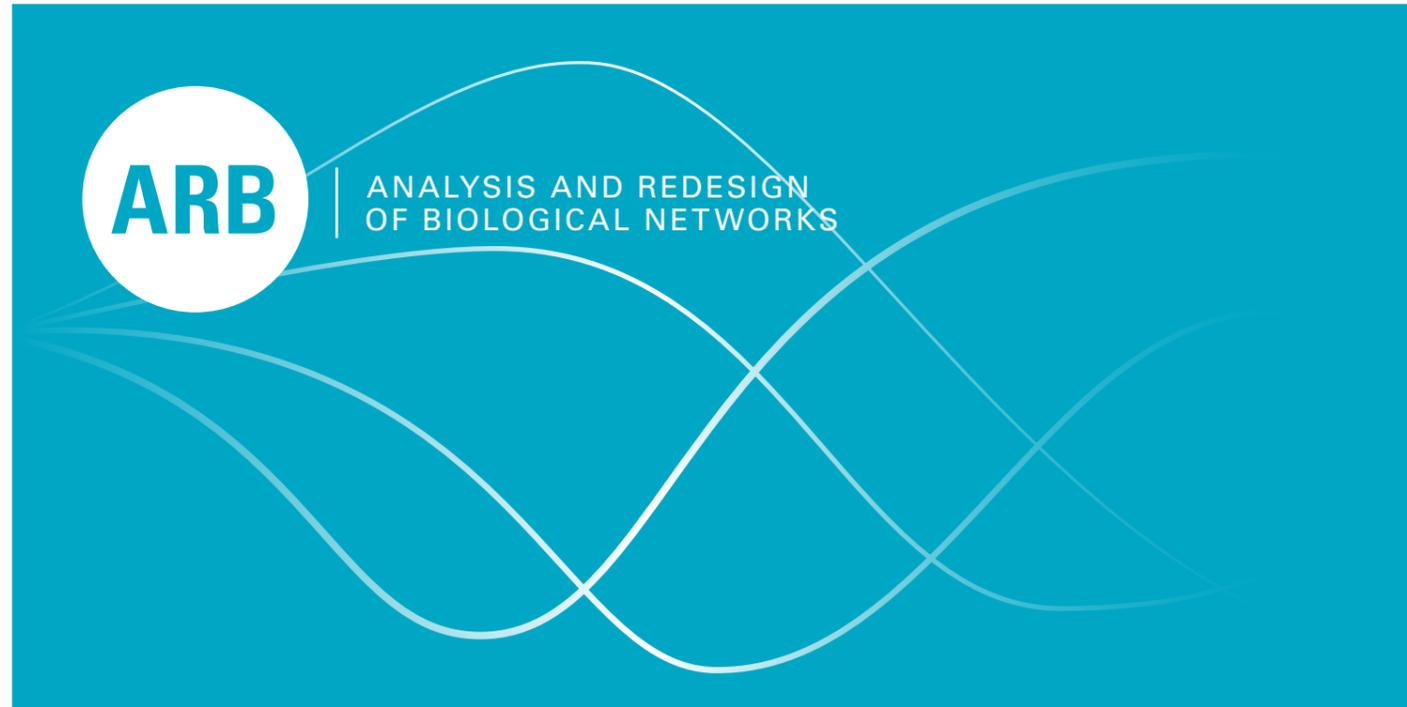
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Author Ion Victor Gosea

Ion Victor Gosea graduated from the Jacobs University Bremen (JUB) in 2011, with a bachelor's degree in electrical engineering and computer science. After continuing with a Master's degree in 2013, he started a Ph.D. project at JUB which he defended successfully in 2017. Since then, he has been a researcher at the MPI Magdeburg. Ion Victor Gosea's research interests include *Model Order Reduction (MOR)* and *Numerical Linear Algebra (NLA)*; in particular data-driven MOR, learning reduced-order models from frequency-domain data, MOR of large-scale dynamical systems, interpolatory and least-square approaches, rational approximation methods. Applications include analysis of models and measured data from *electrical, electro-chemical and mechanical systems*.

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+ Axel von Kamp (left) and Pavlos Bekiaris (right) analyze a metabolic network with their software CNApy, a CellNetAnalyzer-GUI in Python for metabolic network analysis.

DR.-ING. STEFFEN KLAMT | SENIOR SCIENTIST

+ Nowadays, it is widely accepted that understanding the complexity of life at the cellular level requires mathematical and computational tools. Taking this as its research leitmotif, the W2 research group **Analysis and Redesign of Biological Networks** (ARB) develops and applies methods from systems and computational biology and combines them with experimental investigations in order to analyze and rationally modify cellular (biomolecular) networks. One particular focus of our research is the modeling and computational design of metabolic networks in microorganisms with applications in metabolic and biosystems engineering. Other research areas include the theoretical analysis and optimization of microbial communities and of cell-free production systems, as well as the development of comprehensive toolboxes for the computer-aided analysis of biological networks (*CellNetAnalyzer* and *CNApy*).

Apart from theoretical developments, we use various genetic engineering and cultivation techniques to modify and study the physiology of different microorganisms under different conditions. Our experimental studies have a particular focus on *Escherichia coli*, one of the most important model organisms that serves as host in many biotechnological production processes. Another species studied in our lab is *Zymomonas mobilis*, a bacterium with tremendous production capabilities. The tight integration of wet-lab and dry-lab investigations

under one roof enables the prompt implementation and verification of model-based predictions.

Research in our group is thus highly interdisciplinary at the intersection of biology, informatics, mathematics, and engineering sciences. A long-term goal of our activities is to help pave the way for the routine use of advanced mathematical modeling approaches in the life sciences.

Highlights and trends in 2021/2022

Over the past two years, a significant part of our research has centered on the **StrainBooster** project (funded by an ERC Consolidator Grant), which was successfully completed by the end of 2022. This project aimed to establish a new generic principle for rational metabolic engineering of microbial cell factories based on *enforced ATP wasting*. In several case studies, we were able to demonstrate the tremendous potential of the StrainBooster approach. For example, ATP wasting increased the volumetric productivity of a 2,3-butanediol producer strain of *E. coli* by more than 100% and the substrate uptake rate during production under growth arrest by up to 900%. In order to better understand the metabolic response of *E. coli* under high ATP demand, we combined experimental data and model-driven investigations. We found that allosteric regulations in glycolysis lead to a biphasic response of metabolic activity with respect to increasing ATP wasting. This result is key to exploiting the full potential of the StrainBooster approach as it shows that there is an optimal (intermediate) level of ATP consumption

leading to maximal productivity. We are currently in discussions with two biotech companies regarding a possible application of the StrainBooster approach for selected industrial processes.

We also made significant progress in our effort to establish novel genetic tools for *Zymomonas mobilis* that facilitate the exploitation of the extraordinary metabolic capabilities of this bacterium for an extended range of bioproduction processes. In particular, we developed **Zymo-Parts**, a modular toolbox based on Golden Gate cloning for heterologous gene expression in *Z. mobilis*. Zymo-Parts offers a large collection of genetic parts (promoters, terminators, ribosomal binding sites and reporter genes) which can be combined in an efficient and flexible way to achieve a desired level of gene expression, either from plasmids or via genome integration.

Another recently started project in the field of metabolic engineering is **SUPEC**, which is funded by the DFG and headed by our team leader Dr. Katja Bettenbrock together with collaborators from the TU Munich. SUPEC uses systems approaches for advancing production of succinic acid, an important platform chemical, in a two-stage cultivation process with aerobic growth and anaerobic production phases.

Last year, we also announced the first releases of **CNApy** and **StrainDesign**, which are two comprehensive software packages for the analysis and design of metabolic networks,

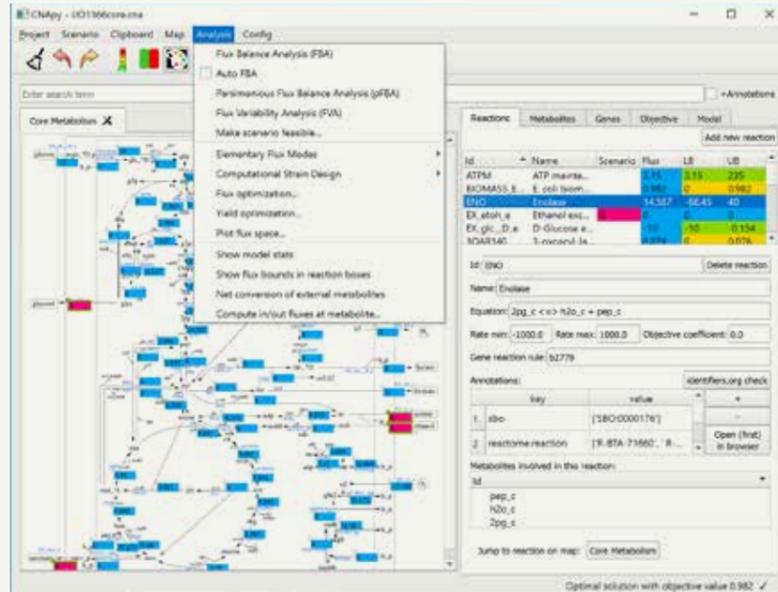
both written in Python. In our Highlight article presented on the following two pages, Axel von Kamp and Pavlos Bekiaris give an overview of these major developments, which offer novel algorithms and a new experience of metabolic modeling on the computer.

In 2021 and 2022, the ARB group published 14 peer-reviewed journal articles and presented its work at several (virtual and in-person) research conferences, including invited talks given by Steffen Klamt at the three major conferences in the field (Metabolic Engineering, COBRA, Metabolic Pathway Analysis). Our group is also grateful for the many interesting and stimulating discussions with the **scientific advisory board** during their (virtual) visit in fall 2021, and we are delighted with the very positive assessment of the research pursued in the ARB group.

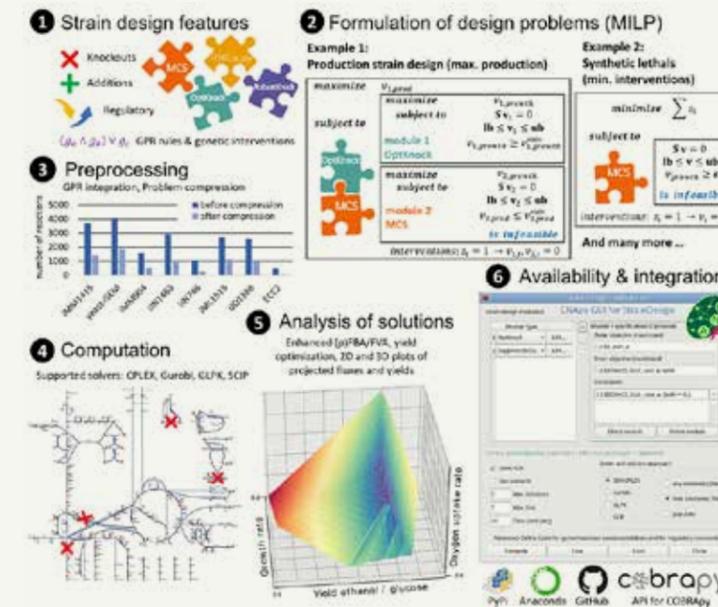
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+ Figure 1: CNAppy with a core model of the *E. coli* metabolism. The fluxes of an FBA solution are shown in the boxes on the map as well as in the table on the right-hand side.



+ Figure 2: Features of the StrainDesign package for the rational modification of metabolic networks.

Powerful Software for the Analysis and Design of Metabolic Networks

Industrial biotechnology is becoming increasingly important for sustainable production processes based on renewable resources. Bioprocesses do not only include traditional fermentations for foods and beverages but also many modern applications, such as the manufacturing of chemicals or pharmaceuticals. Designing efficient bio-based production processes requires a deeper understanding of the microbial metabolism to engineer cell factories with superior production capabilities.

A prominent mathematical method for studying the microbial metabolism is constraint-based metabolic modeling. Here, relevant information on genes, enzymes, biochemical reactions and metabolites is put together in stoichiometric metabolic models, which may comprise thousands of these components. Once such a network model has been reconstructed, it can be used for various computational analyses. Many of these techniques, such as flux balance analysis (FBA), are based on linear programming (LP) or its extension, mixed-integer linear programming (MILP). They aim to simulate physiologic behavior (e.g., growth with maximal growth rate) or to analyze production capabilities (e.g., maximal product yield). Another application is to calculate genetic interventions (strain designs) for metabolic engineering, i.e., the addition or deletion of genes such that the microorganism shows a desired behavior. For instance, one may calculate the interventions needed to ensure that a specified yield of

a desired product is reached. A complementary type of analysis is based on elementary flux modes, which allow one to investigate the various metabolic pathways of a cell, e.g., to identify all possible pathways from a substrate to a product.

CNAppy: interactive metabolic network analysis

Methods of constraint-based metabolic analysis are in widespread use, but there is still a need for user-friendly software that integrates the various techniques in an intuitive manner. For this reason, we developed CNAppy^[1], a Python-based open-source and cross-platform desktop application for metabolic network analysis^[1]. CNAppy (CellNetAnalyzer in Python) adopts the concept of interactive network maps from our previously developed (MATLAB-based) toolbox CellNetAnalyzer (CNA), but advances it in multiple ways. Using Python and the powerful Qt library enabled the implementation of a state-of-the-art frontend with many enhanced features (Figure 1). For example, all genes, reactions and metabolites of a model can be displayed, edited and used to traverse through the network (e.g., from a reaction to all its metabolites and further to all the reactions of those metabolites). Metabolic network maps visualize computational results, greatly helping their interpretation. Various standard and advanced methods and algorithms for metabolic modeling, either developed by ourselves (see also below) or taken from other Python

packages, have been embedded within CNAppy's graphical user interface, and modular extension is facilitated.

StrainDesign: a Python toolbox for computational design of cell factories

One example of a new Python package embedded in CNAppy's GUI is StrainDesign, which was developed in our group^[2] (Figure 2). StrainDesign provides a collection of popular methods for the computer-aided (re)design of metabolic networks that are useful, for example, for engineering microbial cell factories. The toolbox supports several nested strain optimization methods (such as OptKnock) as well as the more general minimal cut sets approach developed in our group^[3]. Advanced features—such as efficient preprocessing, integration of gene-protein-reaction rules and the possibility to combine additions, deletions and up- or down-regulations of genes/reactions—have been generalized and are available for all optimization modules. The package supports multiple solvers and provides various tools for analyzing computed intervention strategies, including

simultaneous projections of selected metabolic fluxes or and product yields. In addition to its user-friendly access in CNAppy, StrainDesign can also be used as a stand-alone package in Python scripts and Jupyter consoles.

CNAppy and StrainDesign are open-source projects and available from their respective GitHub repositories <https://github.com/cnappy-org/CNAppy> and <https://github.com/klamt-lab/straindesign>. CNAppy (and CNA) are also a resource of de.NBI, the German Network for Bioinformatics Infrastructure. **Axel von Kamp, Pavlos Stephanos Bekiaris**

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Author Axel von Kamp

Axel von Kamp studied Biology and Computer Science at the University of Bielefeld. After completing his Ph.D. at Dublin City University, he joined the Bioinformatics department of the University of Jena in 2003. Since 2007, he has been working as a researcher on the development and implementation of algorithms for the analysis of biological networks at the MPI Magdeburg.

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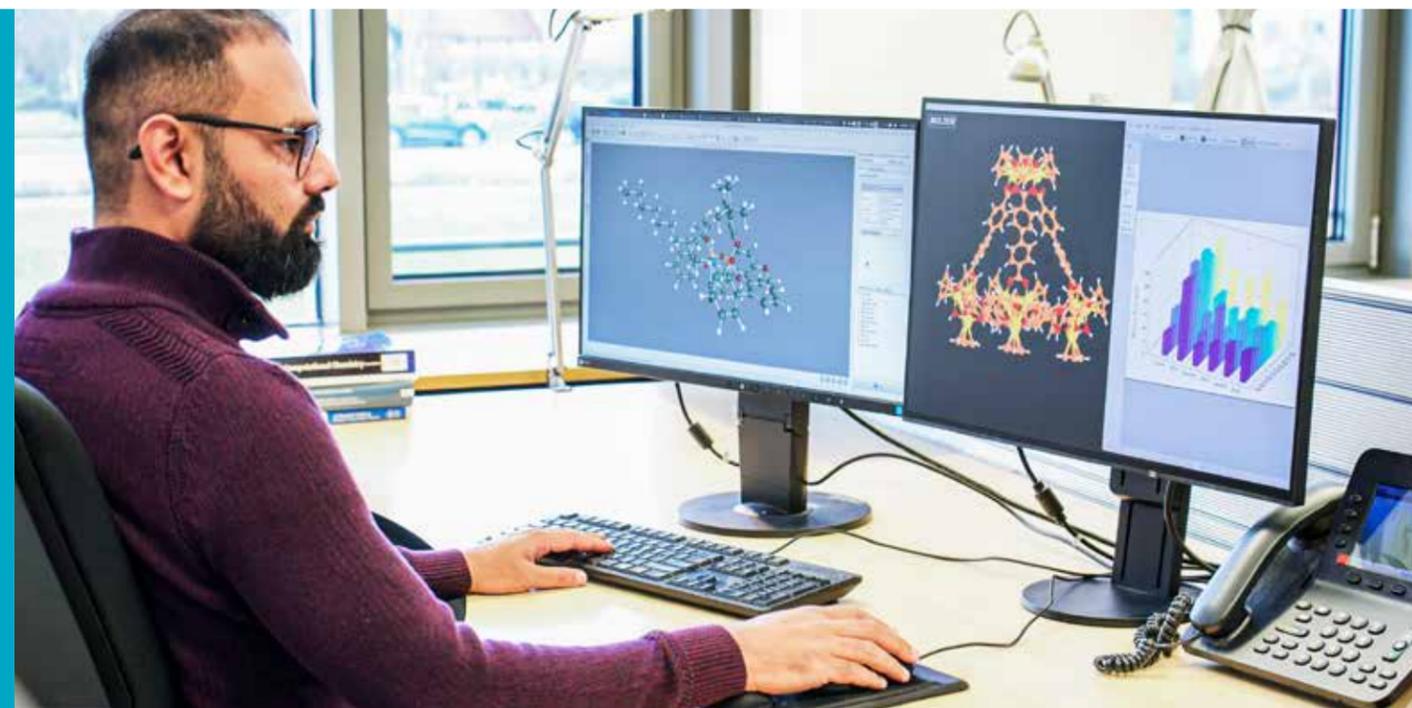
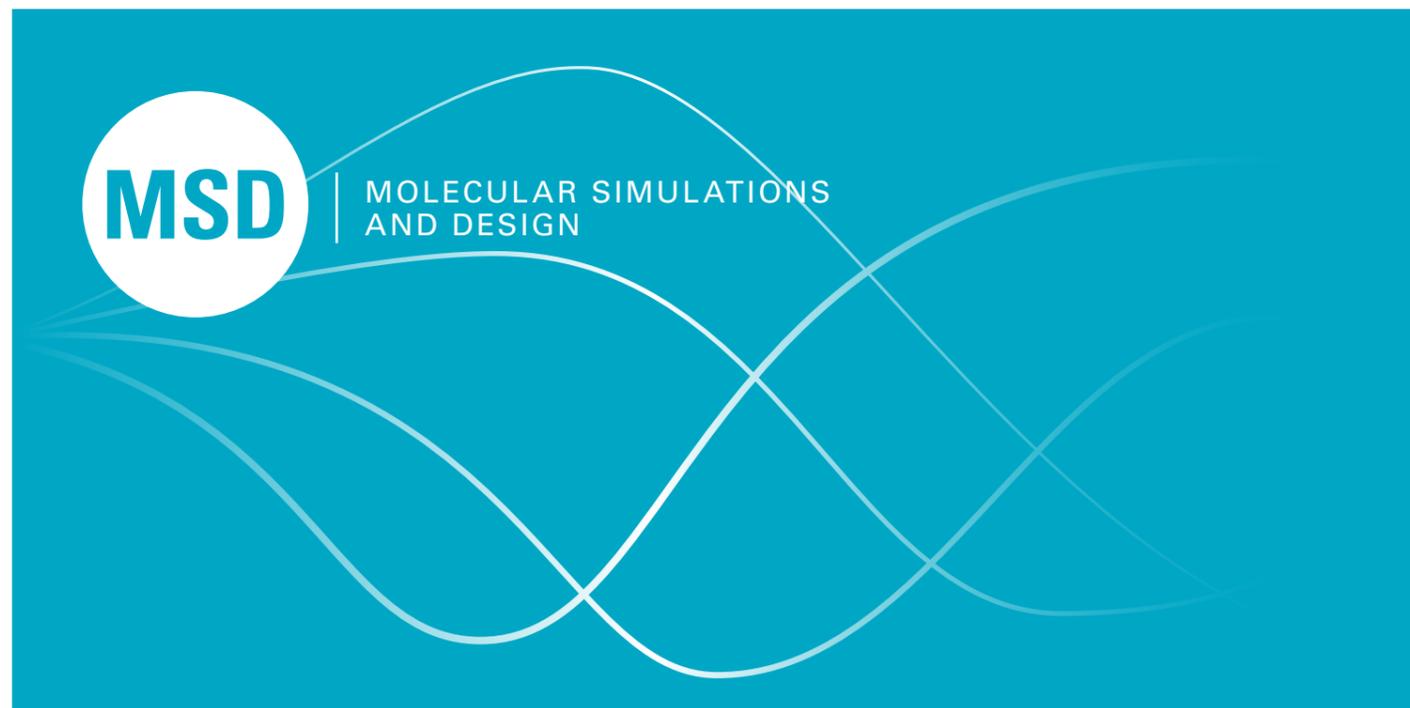


Author Pavlos Stephanos Bekiaris

Pavlos Stephanos Bekiaris studied Molecular Biology (B.Sc.) and Genome-Based Systems Biology (M.Sc.) at the University of Bielefeld and was a visiting student at the University of Manchester. In 2019, he joined the ARB group at the MPI Magdeburg as a Ph.D. student. He develops and implements novel methods and tools for metabolic modeling.

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+ Froze Jameel from the Molecular Simulations and Design group (MSD) designs optimal catalysts and resolves solvent effects at the molecular level for sustainable complex industrial multi-step chemical reactions using quantum chemical methods.

“We have the words to express our anger. We have the words to express our grief. We have the words to express our contempt. We have curse words, words for prayer, we have all the necessary words to talk about ourselves during the war.”

from ‘Three years now we’ve been talking about the war’ (2017)
Serhiy Zhadan (*1974, Ukrainian poet, writer and singer)

PROF. DR. MATTHIAS STEIN | GROUP LEADER

After two years of resilience against SARS-CoV2 in 2020 and 2021 with travelling restrictions, remote working, video conferences and strict means of quarantine and isolation, 2022 was on the verge of getting ways of working and living back to normal. A lot was seemingly back to normal, but everything we were back to doing was harder won - more effort, more worry.

Dr. Meenakshi Joshi was able to join the MSD group in person after a period of remote working from India due to global travel restrictions.

After a very positive and encouraging scientific evaluation of the group by its external Scientific Advisory Board at the end of 2021, the MSD is taking this momentum and verve into the next period of scientific labor.

2022 then turned out to be the hardest year in decades since WWII. The Russian invasion of Ukraine on 24th February showed how valuable and non-obvious it is to be living in peace. War is back in Europe and our thoughts are with our former Ph.D. students, postdocs, and colleagues. Suddenly, scientific contacts and collaborations with Russia are on hold, and Ukrainian scientists are in need of any type of support. The Russian war is also a war on energy, and the need for a rapid transformation process from fossil fuels to renewable energy sources is catapulting our efforts.

The MSD group was hosting Dr. Gözde Yalcin-Özkat, Assistant Professor from the Department of Bioengineering (Rize, Turkey), as a Research Fellow from July 2021 to February 2022. Her stay was supported by a TÜBİTAK fellowship and focused on the use of DFT tight-binding methods to calculate the free energy of ligand-receptor recognition.

2022 also saw Eric Schulze-Niemand defend his doctoral work. In his Ph.D. thesis, he is covering an enormously wide

range of subjects, from post-translational modifications of proteins to the molecular basis for bio-nano hybrid systems. It is the overall dynamics of non-covalent interactions in complex systems that is at the heart of the thesis. The work has led to a number of scientific publications and established new national and international collaborations.

Dr. Ravi Kumar from IIT Bombay is the new 2022 Ernst-Dieter-Gilles Fellow, which is named after the founding director of the MPI Magdeburg. Since July 2022, Dr. Kumar is working in the MSD group on the development of a QM-based workflow to consider microsolvation effects in homogeneous catalysis.

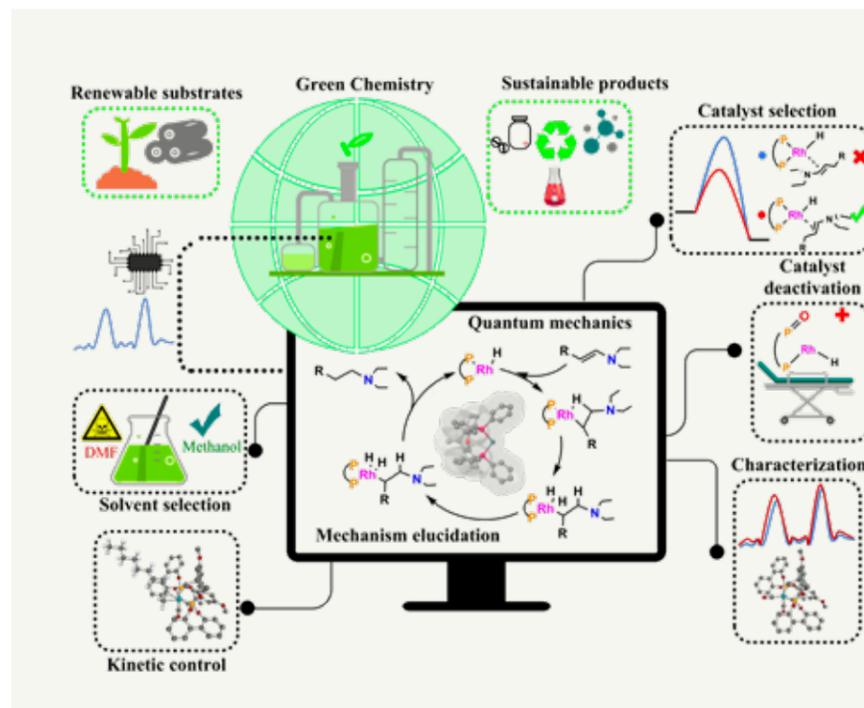
The MSD group has participated in the Collaborative Research Center “InPROMPT - Integrated Chemical Processes in Liquid Multiphase Systems”, supported by the German Research Foundation (DFG), for two periods of funding. Together with scientific partners from OVGU, TU Dortmund, and TU Berlin, bio-based alternatives as commercial sources of supply for polymer raw materials from long-chain fatty acids and vegetable oil methyl esters have been investigated. The catalytic systems consist of advanced transition metal catalysts with sophisticated multi-dentate ligands, which are designed to provide the desired product in high yield and purity. Computational chemists often use a truncated model system to describe such complicated catalytic processes. We chose to

go another way and treat the full system quantum mechanically after carefully benchmarking the accuracy of current state-of-the-art methods. All atoms are incorporated at the same level, thus avoiding artefacts from unbalanced basis sets or QM/MM approaches. The consideration of the effect of solvents or solvent mixtures has revealed their effects on chemical equilibria and kinetics and indicated points of control and intervention. The explicit modelling of solvation becomes critical for coordinating solvents when there is the possibility of a direct interaction between solvent and catalyst. Such insight directly enters the design of experiments and cannot be obtained from other computational solvent-screening approaches.

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+ **Figure 1:** Computer-aided rational design of catalysts and solvents in industrial homogeneous multi-phase processes.

Rational Design of Green Solvents for Homogeneous Multi-Phase Reactions

The chemical industry provides us with high-end products, from pharmaceuticals to commodity chemicals, which make our lives much easier and more comfortable. However, in response to global warming and climate changes, a swift transition from the wide and cheap availability of fossil fuels to substrates from renewable sources instead of fossil fuels is necessary.

To achieve this goal, alternative processes that follow the general guidelines for green chemistry must be developed. Non-toxic solvents, highly selective catalysts, and advanced process intensification methods are some screws that we can turn (see Figure 1).

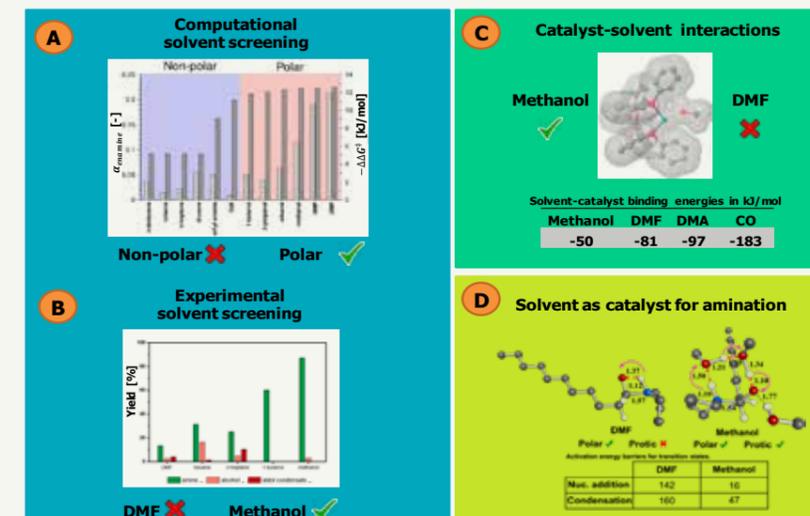
Our computer-aided rational design approach working towards the development of more sustainable processes starts with an exploration of the potential energy surface along the reaction mechanism using quantum mechanical methods. These potential energy surfaces show the pathways of the main reaction plus all side reactions and provide the thermodynamic and kinetic parameters of large-scale industrial chemical processes. The molecular and atomistic insight into the reaction mechanisms enables the development of highly active and selective catalysts with a high yield, thus reducing side product formation and leading to more economically efficient processes. By fine-tuning appropriate conditions, the productivity and selectivity of such

processes can be controlled according to the choice of solvent and external parameters such as temperature and pressure.

A solvent plays many roles in a chemical reaction, e.g. solubilization of substrates, catalyst, and products; as a reaction medium; as a substrate or co-catalyst itself; or as a product separation agent. The choice of solvent also affects the reaction pathway, chemical reaction equilibria, and transition state barriers and thus alters the thermodynamics and kinetics of the reaction. Solvent molecules may explicitly interact with the catalyst, the substrates and products, and transition states and can affect the process rate and/or its selectivity.

In the interdisciplinary CRC/Tr63 “InPROMPT”, a range of complex reaction mechanisms with relevance to greener industrial processes (hydroformylation¹, reductive amination^[2] and hydroesterification^[3]) were investigated in collaboration with experimental partners at TU Dortmund and OVGU. In these homogeneous transition metal catalyzed reactions, the solvent dependence of reaction equilibria and rates of reactions was probed. Investigations of possible side reactions allowed the rational control of the catalysts’ selectivity towards the desired products. Along the potential energy surfaces, the rate-determining steps could be identified. They enter directly into the design of microkinetic models^[4, 5] and are describing the kinetic control of the reaction.

Computational solvent design



+ **Figure 2:** Computational solvent design: A) solvent screening and activity coefficients for the rate determining step for a set of solvent candidates, B) experimental validation for a sub-set of solvents, C) modeling explicit catalyst-solvent interactions, D) the role of solvent as a co-catalyst.

As an example, the reductive amination of undecanal from fennel with diethylamine to give the (bio)-polymer polyamide PA11 building blocks is presented. Exploration of the potential surface has identified the Rh-catalyzed reduction step of the amination to be rate-limiting.^[2] In a first fast screening of the effect of the dielectric constant on the reaction rate ($\Delta\Delta G^\ddagger$), polar media showed good performance by lowering the transition state barrier. Implicit solvent models do not take the non-ideal behavior of solvent into account, which can be included via calculations of the activity coefficient (α) of the intermediates in solution. Screening of the enamine activity coefficient in various solvent candidates gave consistent results with QM: dimethylformamide (DMF) was top-ranked, followed by NMP and methanol (see Figure 2 (A)). However, a clear solvent discrimination cannot be made based on these initial criteria only.

Based on the computational ranking, experiments for a subset of representative solvents were conducted. Although DMF was found to be one of the most promising solvents, experimentally it showed the lowest product yield (see Figure 2 (B)).^[6] Such an unexpected effect could only be explained by explicitly modeling the catalyst-solvent interactions. A strongly coordinating solvent can, for example, inhibit substrate binding and thus deactivate the catalyst in the process. Weak catalyst-solvent interaction is thus desirable for a high catalytic activity.

According to our results, DMF itself was found to be a strong coordinating solvent to the catalyst, but also its thermal decomposition products (CO and dimethylamine) were inhibiting and deactivating the catalyst. Methanol as an alternative with similar polarity to DMF, on the other hand, does not only have significantly less ecological impact but is also a relatively weak coordination agent. Thereby, substitution of DMF with methanol will significantly increase the catalytic activity during the reductive

amination process (Figure 2 (C)). Methanol as a hydrogen bond forming solvent is furthermore highly advantageous as it also acts as co-catalyst during amination. It significantly reduces the transition state barriers compared to polar DMF (see Figure 2 (D)).

In summary, quantum chemistry can be a powerful tool in designing appropriate solvents for catalytic transformations. It significantly reduces the number of time-consuming experimental solvent screenings in the development and optimization of green and sustainable processes that transform renewable substrates into valuable chemicals. | **Froze Jameel**

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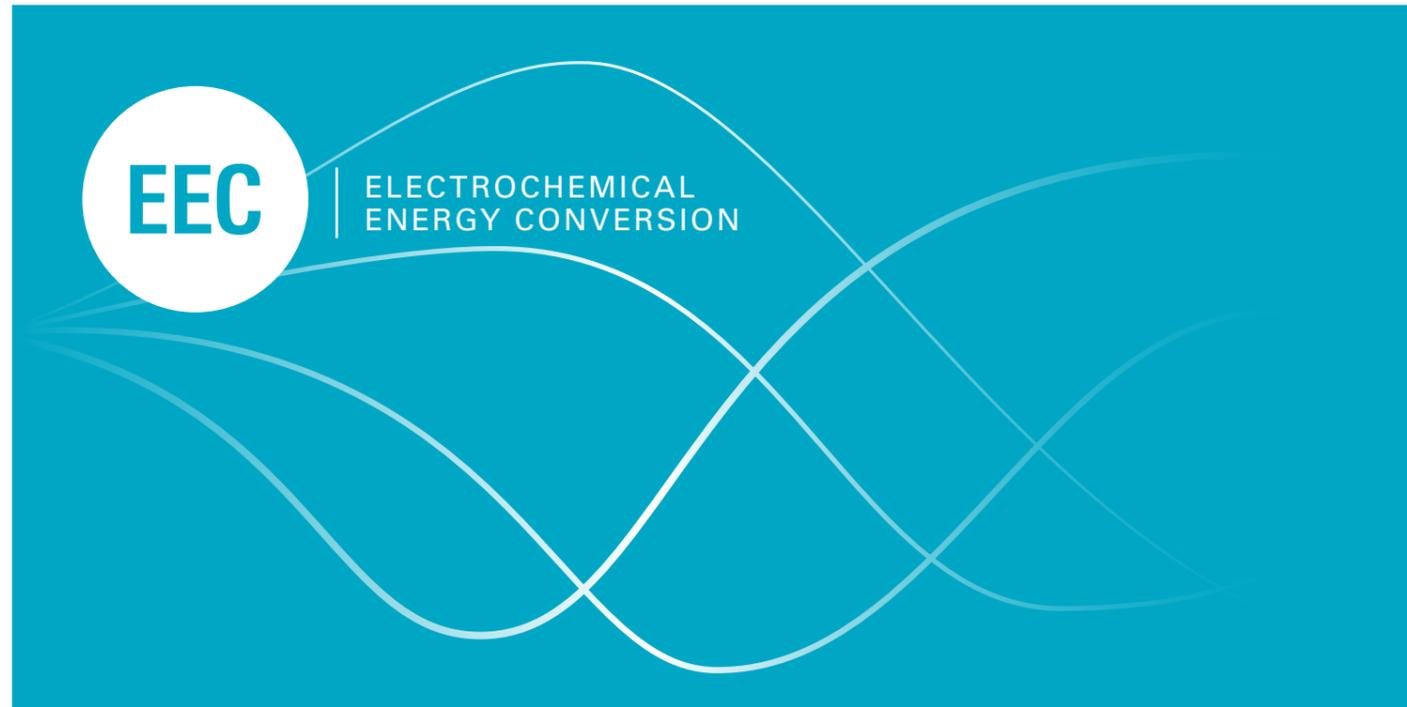
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EEC | ELECTROCHEMICAL
ENERGY CONVERSION



+ IMPRS doctoral candidate Tamara Miličić and her Master student Thanh Hoang Vu are performing experiments on the proton exchange membrane water electrolysis test bench.

DR.-ING. TANJA VIDAKOVIĆ-KOCH | SENIOR SCIENTIST

Electrochemical process engineering is becoming a key discipline in the context of the energy transition and the associated electrification of industry and transport (electromobility). The key technology in this context is water electrolysis, which enables renewable and volatile electricity from wind and solar energy to be stored using hydrogen. Hydrogen has the potential to defossilize various industries (such as ammonia or steel production), transportation (especially heavy vehicles), and also heating. In addition, there is great potential for the development of further electrochemical processes in which various value-added products can be synthesized using renewable electricity, (bio)waste, carbon dioxide and nitrogen. In all these applications, the dynamic and volatile nature of renewable energy forces dynamic operating conditions for electrochemical processes. Therefore, understanding of dynamics of electrochemical processes is of high interest.

Dynamics of electrochemical processes

Different aspects of dynamics of electrochemical processes are currently studied. In kinetics, our focus is on understanding oxygen and carbon dioxide reduction reactions on silver under alkaline conditions. This project is being under-

taken within the framework of a large research network of the German Research Foundation (FOR 2397) involving a total of seven university and non-university academic partners. The aim is to improve understanding of reaction and transport processes in gas diffusion electrodes (GDEs). In September 2022, the EEC group, in collaboration with partners from DFG Research Group 2397, organized a second International Symposium on Gas Diffusion Electrodes in September 2022 in Magdeburg. As at the first event in 2019, many outstanding plenary and guest speakers made the symposium a great success. Although GDEs are used in various processes, it became clear during the GDE symposium that CO₂ reduction was of particular interest.

In water electrolysis our particular interest is on understanding of an impact of mass transport losses on water electrolysis efficiency. This work is described in more detail in our research highlight by Tamara Milicic.

Data-driven modeling is an emerging direction in several areas of science and the EEC group is developing its interest in this direction. Here, we are collaborating with the DRI group at MPI. The DRI group, led by Prof. Antoulas, has developed a tool called the Lowener framework for data-driven analysis of frequency response data in the linear domain. We are currently applying LF to several types of data measured in our labs or by partners. It is clear that a data-driven approach requires a large amount of data. A particular chal-

lenge seems to be to assign the resistances determined by LF to a specific physics of the system. Here, in addition to data, correlation with physics-based mathematical models and machine learning tools seems to be a promising direction.

Bioelectrochemical processes

We aim to develop new electrochemical processes in which redox enzymes are used instead of traditional metal catalysts. This is a promising direction, but also challenging. We address different challenges on electrode and enzyme sides in our joint project with Bornscheuer's group at the University of Greifswald within the framework of the DFG Priority Program "Bioelectrochemical and Engineering Fundamentals to Establish Electro-Biotechnology for Biosynthesis – Power to Value-Added Products (eBiotech) – SPP 2240".

Electrochemistry meets synthetic biology

We work on the development of artificial organelles in the context of bottom-up synthetic biology. Here, I would like to highlight a research paper by Lado Otrin as lead co-author, published in Nature Communications, in which he showed that more complex artificial "respiratory chains" can be built using some smart strategies invented by nature. In particular, a so-called SNARE protein could be used to build complex, fully artificial systems. The mechanism of fusion with hybrid and polymer vesicles was visualized for the first time.

Defences and more

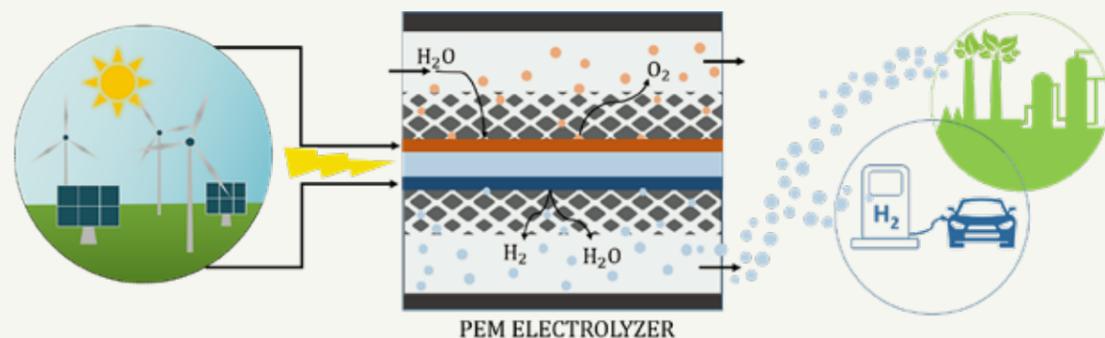
A growing interest in electrochemical technologies is also reflected in the number of students showing interest in this topic at Otto von Guericke University. In the 2022 summer semester, almost 200 students registered for the fuel cell technology exam.

In 2021, three group members defended their Ph.D. theses. Our new group member, Mohammed Al-Saif Al-Shaibani, is the best international student of Faculty of Process and Systems Engineering at OVGU. We congratulate him and look forward to working with him in the group.

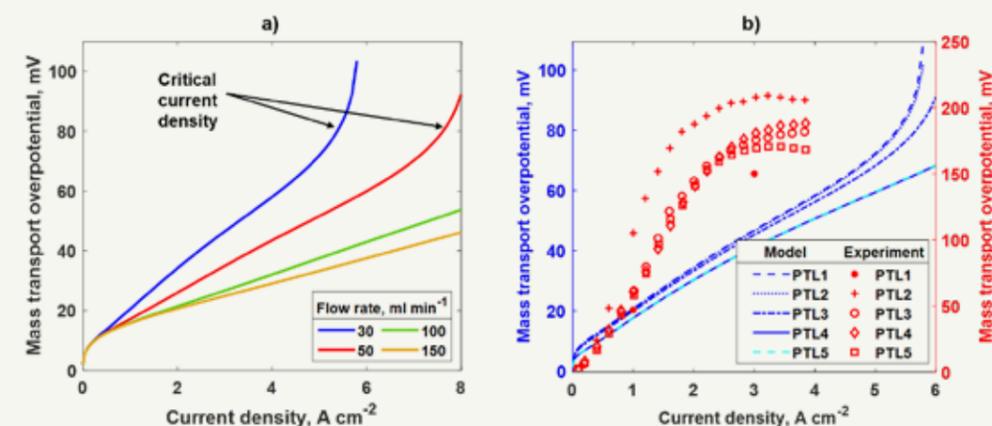
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+ **Figure 1:**
Schematic representation of green hydrogen economy with PEM electrolyzer as main technology for hydrogen production



+ **Figure 2:**
Mass transport overpotential as function of current density for a) different inlet water flow rates and b) different PTL structures^[1,3]

Towards Efficient Green Hydrogen Production: PEM Water Electrolysis

Growing energy crises and severe climate changes have shifted the economy transition away from fossil-based fuels towards sustainable technologies. Green hydrogen has emerged as a favorable alternative to fossil fuels in the industry, transportation, and energy sectors. By coupling proton exchange membrane (PEM) electrolyzers with renewable energy sources, it is possible to produce high-purity hydrogen completely emission free (Figure 1). Bearing in mind the importance of PEM electrolyzers for decarbonization and the sustainability of the economy, there is huge pressure to further improve the performance and lifetime of these devices. As learned from the past, this will be possible only with profound theoretical understanding of phenomena governing PEM electrolyzer operation.

Multiple phenomena occur simultaneously in the PEM electrolyzer: water oxidation to oxygen at the anode, hydrogen evolution at the cathode, two-phase transport of water and produced gases, proton transport through the PEM, etc. The complex coupling of the different processes determines electrolyzer performance. To minimize losses, improve durability, and increase productivity, a fundamental understanding of these processes is needed, but is still lacking. Experimental investigation results in substantial information about the electrolyzer's performance. However, it is quite challenging and time inefficient to identify experimentally individual phenomena

resulting in voltage losses. Here, mathematical models are an invaluable tool. While microscale and mesoscale models provide information about the processes occurring on a smaller scale, macroscopic models are essential for studying electrolyzer performance as a whole. Combining information from different scales can enable more realistic performance prediction. This approach was utilized here in order to understand the origins of mass-transport losses in water electrolysis^[1,2].

First, a macroscopic dynamic model was developed coupling two-phase transport in the anode porous transport layer (PTL) and electrochemical half-reactions [1]. The model is based on the following assumptions: i) counter-current mass transport of water and oxygen produced at the anode PTL is slow and oxygen is accumulating in the pores of the anode PTL; ii) due to this, water cannot reach part of the catalyst and the oxygen evolution reaction is inhibited; iii) finally, this results in the mass transport overpotential which contributes to electrolyzer efficiency decrease. In the model, mass transport overpotential is calculated by taking into account the part of the active area that is covered with gas. The multiphase mass transport submodel describing two-phase transport in the PTL is employed for the determination of the liquid and gas fractions in the PTL. The gas fraction at the interface between PTL and the anode catalyst layer is taken to be equal to the gas fraction on the active area.

The macroscopic model obtained was used for studying the influence of current density, inlet water flow rate, and PTL structure on the mass transport overpotential. It was found that an increase in current density results in the filling of the active area with gas and an increase in mass transport overpotential (Figure 2. A). When the electrode surface area is almost completely covered with gas, the mass transport overpotential increases exponentially. The current density under these conditions is termed critical current density. At slightly higher values than the critical current density, the reaction stops. Inlet water flow rate had the opposite effect to current density: an increase in the flow rate decreases the mass transport overpotential and increases the critical current density (Figure 2. A). To understand the effect of the PTL structure on the two-phase transport, pore network modeling (PNM) was implemented. It was shown that PTL structure has an important effect on mass transport through the PTL and graded PTL was found to facilitate it^[2]. This is in accordance with the results of the macroscopic model, which confirmed that mass transport overpotential can be lowered by choosing the optimal PTL structure (Figure 2. B). High porosity, wide pore size distribution, and large pores result in lower mass transport overpotential. Additionally, a significant improvement in electrolyzer performance is predicted for graded PTL^[1].

Even though the modeling results are in agreement with experimental data in the literature^[3], some differences were observed (Figure 2. B). At low current densities, the experimental data shows a linear increase in mass transport overpotential, while the model predicts an exponential rise. The difference observed can be due to the approximate nature of the methods used for experimental mass transport overpotential determination. This demonstrates a necessity to use

mathematical models for the interpretation of experimental data, which is the focus of our future work. Additionally, further model improvements by using information obtained at mesoscale with PNM, as well as dynamic analysis, will contribute to better prediction capacity of the model. Finally, an advanced tool for PEM electrolyzer diagnosis is targeted^[4].

Tamara Miličić

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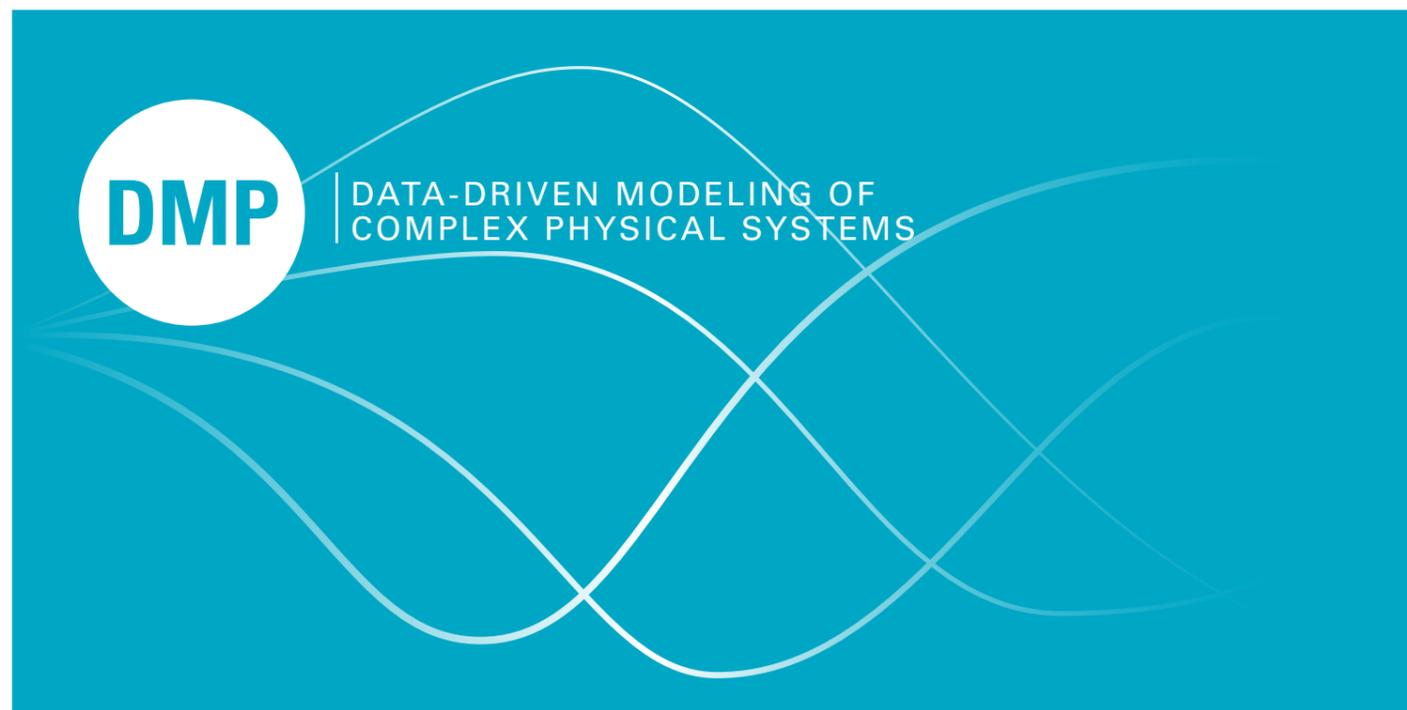
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Tamara Miličić studied at the Faculty of Technology and Metallurgy, University of Belgrade, Serbia, where she received her Master's degree in Chemical Process Engineering in 2019. In 2020, she started her Ph.D. studies in the Electrochemical Energy Conversion group at Max Planck Institute in Magdeburg as part of the IMPRS ProEng program. Under the guidance of Dr-Ing. Tanja Vidaković-Koch, she is investigating the performance of the proton exchange membrane electrolyzer by employing a combination of mathematical modeling and experimental analysis.

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+ Mathematician Dr. Feliks Nüske analyzing molecular dynamics simulation data using the DMP group's own software.

DR. FELIKS NÜSKE | SENIOR SCIENTIST

The DMP Group was formed in April 2022 with the goal of strengthening the MPI's research activities in the field of data science, geared towards physical systems on the molecular scale.

Research Scope

Computer simulations have become an essential tool to aid our understanding and our ability to predict or manipulate complex systems ranging from atomistic to macroscopic scales – from the quantum properties of single molecules to atmospheric flows. Among the major impediments to the routine use of computer models, the following three challenges can be identified: **high-dimensionality, vast timescale gaps, and modeling errors**. The first issue refers to the overwhelming number of degrees of freedom required to describe a system. For atomistic simulations of macromolecules, this number equals three times the number of atoms in the system, which can easily exceed several hundred thousand. The second issue refers to the presence of many different characteristic timescales, which often separate elementary integration time steps from timescales of scientific interest by many orders of magnitude. The third issue

captures the problem that many computational models are simplifications of an accurate but computationally infeasible ground truth model, leading to inherent model uncertainty.

The goal of the DMP Group is to tackle these problems by leveraging the dramatic progress made over the last two decades in the field of data science in order to arrive at efficient analysis and modeling tools which respect the physics of the system under investigation. A particular focus of the research in our group is mathematical analysis of the proposed methods, addressing questions of convergence, robustness, and computational cost.

Research Goals

Our research revolves around **Koopman operator theory**, which offers a statistical description of a dynamical system in a feature space of observation functions. The main technical advantages of the Koopman approach are, first, the dynamics in the feature space are linear, and second, a discretization of the feature space dynamics can be estimated from simulation data using machine learning methodology. Our work builds on these advances by investigating the following questions:

Discretization: Numerical discretization of the Koopman operator requires a finite dictionary of observation functions. In the past, these have often been designed manually based

on intuition or prior knowledge. In our work, we aim to build dictionaries which are largely model-agnostic and therefore more transferrable across systems. We focus on **reproducing kernels** and **low-rank tensor approximations**, and seek to design new algorithms and analyze their mathematical properties, allowing for the efficient and robust analysis of large-scale systems that were previously inaccessible to numerical treatment.

Model Reduction: As alluded to earlier, high resolution models of a system are often very expensive to simulate. At the same time, having access to all the detailed information they contain may not even be relevant for practitioners. Therefore, reduced models are of paramount importance across all disciplines. As the Koopman operator contains virtually all statistical information about a system at hand, it can also be used to learn **reduced models** from existing simulation data. With the tools developed in our lab, these models can be estimated efficiently and transferred across models effectively. On the first two topics, there is ample opportunity for collaborations with the CSC group.

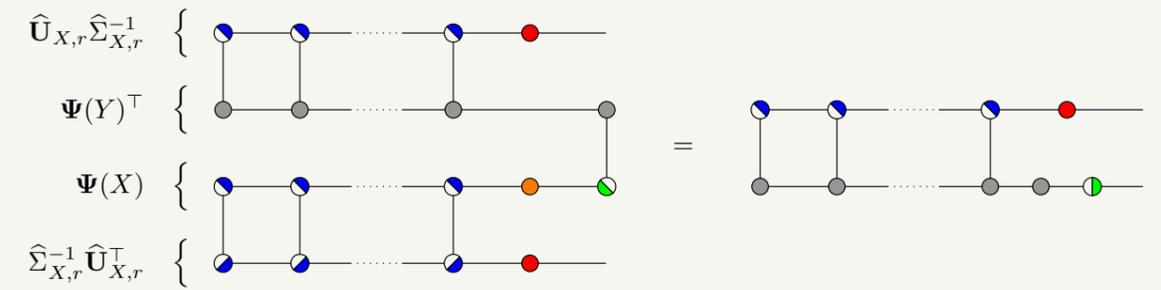
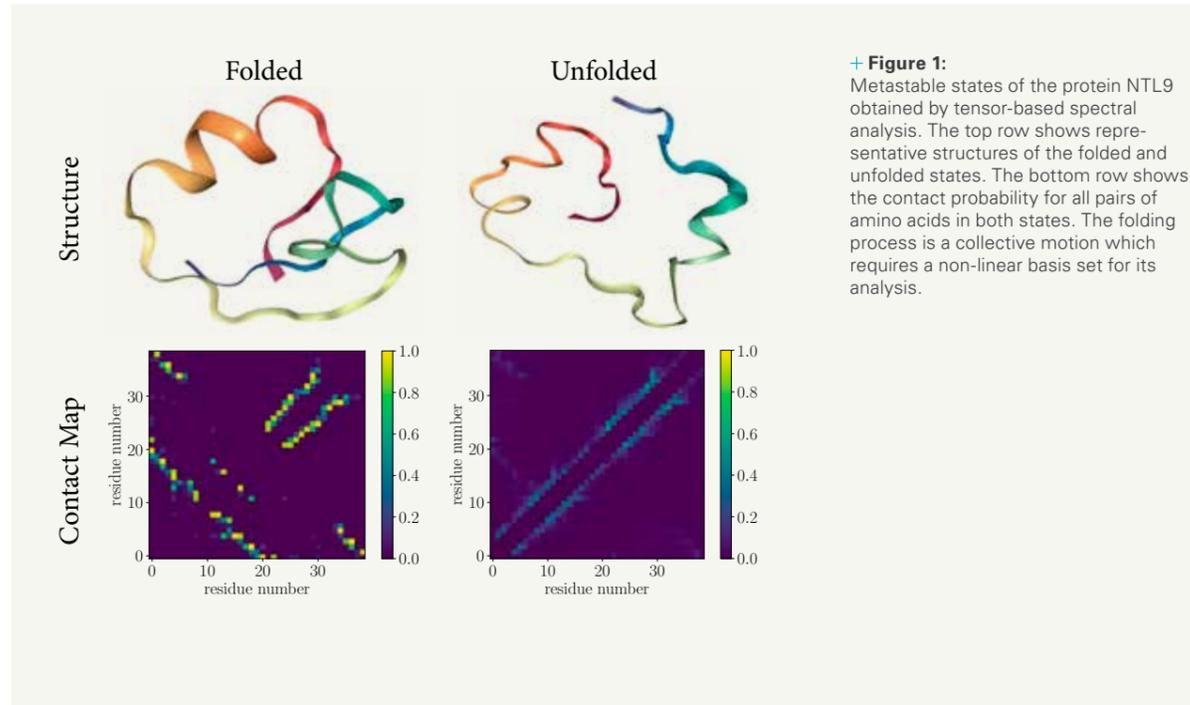
Molecular Applications: The guiding application for our research is **high-resolution simulations of macromolecules** (MD simulations). These have been used successfully in many areas of physics, chemistry, and biology. Our methods are built to facilitate the analysis and model valida-

tion process for molecular simulations. They will also allow for the efficient parametrization of reduced models, allowing bridging between different levels of resolution. In a recent development, we have also applied our methods to analyze quantum systems. We anticipate close collaborations with the MSD group in this area.

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Tensor-Based Analysis of Metastable Dynamical Systems

+ Metastability is a prominent feature of dynamical systems in various scientific fields. The term refers to the existence of a few regions in the system's configuration space where the system spends long periods of time before occasionally transitioning into another such region. The transition times are much faster than typical residence times within the metastable states. A prime example of this phenomenon is given by computer simulation models of biological macromolecules. Metastable states could then, for example, correspond to different bound and unbound states of a molecular complex.

Metastability is a major impediment to the routine application of computer simulations to complex systems as it increases the amount of simulation data required for a robust analysis far beyond what is feasible on state-of-the-art machines. At the same time, characterizing metastable states—and the rates of transition in between them—is a very important objective for practitioners. Coming back to the example above, identifying different bound and unbound states for a molecular target/inhibitor complex is of central importance in the drug development process.

Koopman Operators

Mathematically, metastability is reflected in the spectrum of a family of linear operators, called **Koopman operators**^[1]. These operators describe the time evolution of expectation values of

functions on state space, called **observables**. If the dynamical system is metastable, one can expect a cluster of eigenvalues close to one, separated from the remaining spectrum by a spectral gap. Analysis of these leading spectral components allows metastable states and transition rates to be identified.

Numerical approximation of the Koopman operator is achieved using a projection onto the linear space defined by a finite basis, called **dictionary**. Choosing the right dictionary is crucial in practice and involves expert knowledge and intuition. Once the dictionary is fixed, the projected Koopman operator can be estimated using simulation data^[2]. This fact has been at the heart of the remarkable success of the Koopman approach in recent years: as long as sufficient data is available and a good dictionary can be defined, the underlying dynamical system can be successfully analyzed, even if its equations of motion are not known in closed form.

Tensor Product Formats

To address the problem of dictionary selection, a widely used approach is to first define several elementary dictionaries, for instance, univariate functions of a single state variable. A large dictionary is then formed by including all possible products of elementary functions. This is an example of a **tensor product representation**, as the product functions can be represented by multi-dimensional arrays (tensors). In

a brute-force approach, the number of parameters required to represent such a tensor scales exponentially with the number of elementary subspaces. However, in many cases, there is at least persuasive evidence that much fewer parameters are actually needed to obtain an approximate representation of the tensor. Systematic ways of parametrizing tensors at low complexity are known as **tensor formats**. A particularly intuitive and mathematically rich example is the **tensor train (TT)** format^[3].

Tensor-Based Koopman Approach

In this project [4, 5], we employed the tensor train format to efficiently compute the Koopman operator using a product basis as described above. The fundamental insight was that all data-based quantities required by the Koopman approach are endowed with an exact TT representation due to the product structure of the dictionary. The complexity of these representations is governed by the data size alone. In addition, the TT representations can be truncated in a controlled manner using well-known procedures developed by the numerical linear algebra community. Finally, we showed that calculation of the Koopman spectrum can be cast as a standard matrix eigenvalue problem. The reduced matrix can be computed efficiently by exploiting the TT structure of all quantities involved. In summary, our approach allows approximation of the Koopman spectrum using large, relatively uninformed dictionaries using efficient low-rank representations. The computational cost of the approach is dictated by the simulation data.

Application to Molecular Systems

We validated our approach using two benchmarking examples of atomistic molecular dynamics simulations, namely

the deca-alanine peptide and the 35-amino-acid protein NTL9. For both systems, we were able to show that efficient representations of the Koopman operator could be inferred from the simulation data. The spectral analysis of the resulting reduced matrix allowed recovery of the dominant metastable states and their transition rates, which correspond to folded and unfolded states in both cases.

| Dr. Feliks Nüske

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+ Publications 2021

Journal Articles

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