

## ENTRY FEES/REGISTRATION

### – Entry fees

- Industry: 690 EUR\* (presence) 200 EUR (online)  
(VAT is not charged according to § 4 No. 22a UStG)  
Invoicing takes place after the event.
- Research staff: free of charge (presence and online)

\*During the event, coffee, refreshments and lunch will be offered. Registered participants will receive the workshop documents, a certificate of participation and can attend the networking dinner on September 30, 2021.

### – Registration

This year's workshop will take place on site in Kaiserslautern – under consideration of the applicable distance and hygiene rules – and online offer.

Please register online by **September 20, 2021**:  
[www.leistungszentrum-simulation-software.de/mmipe21](http://www.leistungszentrum-simulation-software.de/mmipe21)



## GENERAL INFORMATION

### – Contact with regard to scientific program

**PD Dr. Michael Bortz**  
Department Optimization – Technical Processes  
Fraunhofer Institute for Industrial Mathematics ITWM  
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[www.itwm.fraunhofer.de](http://www.itwm.fraunhofer.de)

### – Contact with regard to organization

**Sylvia Gerwalin**  
Phone +49 631 31600-4424  
[sylvia.gerwalin@itwm.fraunhofer.de](mailto:sylvia.gerwalin@itwm.fraunhofer.de)


### – Conference venue (on site participation)

**Fraunhofer Institute for Industrial Mathematics ITWM**  
Fraunhofer-Platz 1  
67663 Kaiserslautern  
[www.itwm.fraunhofer.de](http://www.itwm.fraunhofer.de)

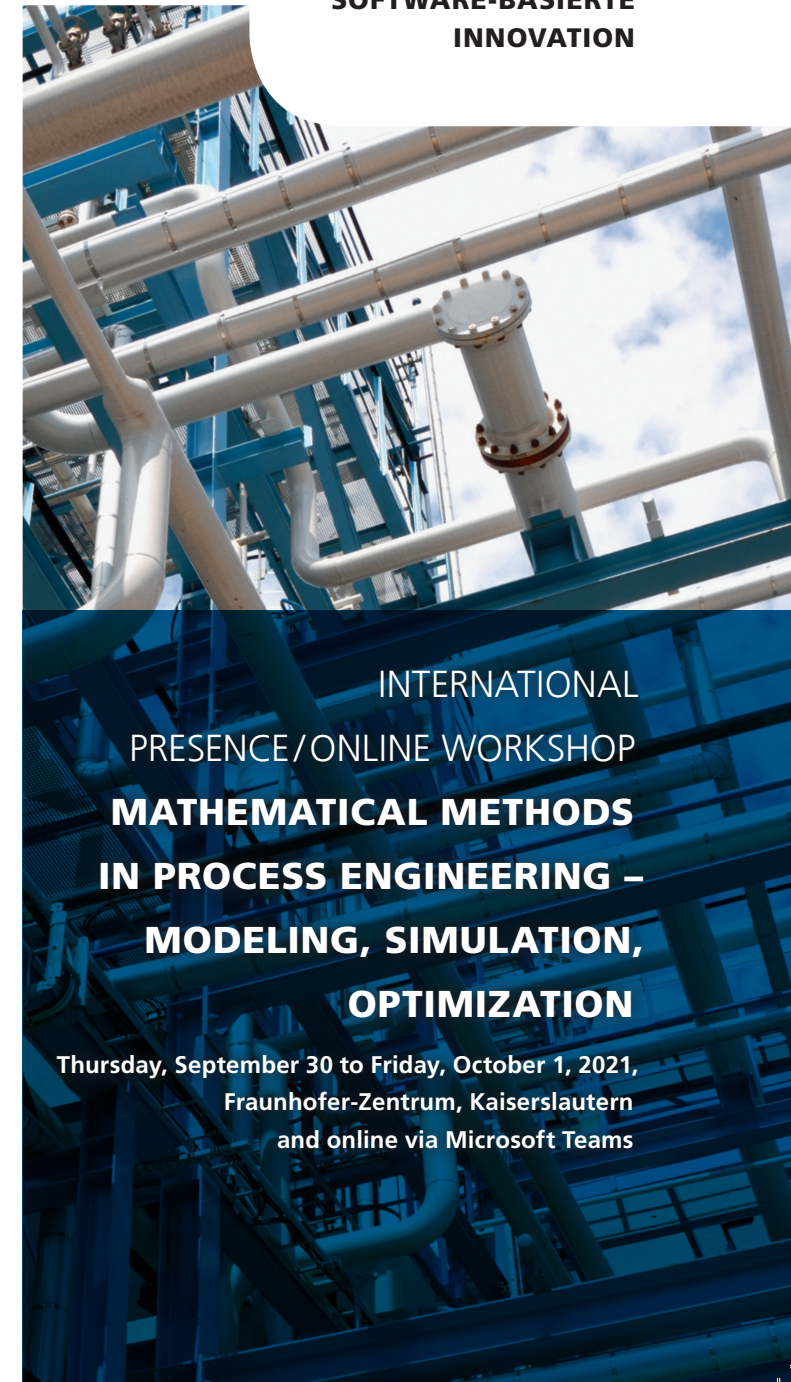
Directions: [www.itwm.fraunhofer.de/en/contacte](http://www.itwm.fraunhofer.de/en/contacte)

### – Conference software (online participation)

The event will also take place in the form of a video conference with Microsoft Teams. You will receive an access link a few days before the workshop, which you simply click on.



LEISTUNGSZENTRUM  
SIMULATIONS- UND  
SOFTWARE-BASIERTE  
INNOVATION



## PREFACE

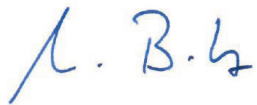
Model-based simulation and optimization is considered an essential ingredient for unveiling potential for increased energy and resource efficiency as well as for maintaining a high level of value creation.

Mathematical models, algorithms and data science are in the core of this development.

In fall 2021, September 30 to October 1, the Fraunhofer High Performance Center Simulation and Software-based Innovation will organize an international presence and online workshop “Mathematical Methods in Process Engineering – Digitization in the Chemical Industry” with 6 internationally outstanding invited speakers and 12 short contributions from researchers of the center and industry.

All lectures are invited, and also attendance will require invitation.

The number of invited participants is limited to about 80, which will include selected partners from process industry as well. The workshop will provide a unique opportunity for scientific discussions and personal networking between scientists from academia and industrial practice to render and to shape the topics to come in future process engineering.



PD Dr. Michael Bortz  
Fraunhofer ITWM



Prof. Dr.-Ing. Hans Hasse  
TU Kaiserslautern

## PROGRAM – THURSDAY, SEPTEMBER 30

9:45	Registration open, welcome coffee
10:00	<b>Opening</b> PD Dr. Michael Bortz, Prof. Dr.-Ing. Hans Hasse
10:15	<b>Opening Keynote</b> Dr. Rainer Lemke, BASF SE
<b>S1: MSO FOR DYNAMIC PROCESSES I</b> Session Chair: Prof. Dr. Karl-Heinz Küfer	
10:45	<b>Flexible Chemical Industry: From Scheduling to Online Optimization</b> Prof. Alexander Mitsos, PhD, RWTH Aachen
11:35	<b>Dynamic Modeling, Simulation and Optimization in Process Development</b> Dr. Norbert Asprion, BASF SE
12:00	<b>Rapid Prototyping for Model-based Comparison of Control Schemes</b> Dr. Jochen Schmid, Fraunhofer ITWM
12:25	Lunch (foyer)
<b>S2: FILTRATION AND SEPARATION</b> Session Chair: Prof. Dr.-Ing. Hans Hasse	
13:30	<b>Multiscale Simulation and Control of Centrifuges in Process Scale</b> Prof. Dr. Hermann Nirschl, Karlsruhe Institute of Technology (KIT)
14:20	<b>Simulation-based Optimization and Characterization of Woven Filter Screens</b> Dipl.-Ing. Markus Knefel, GKD – Gebr. Kufferath AG
14:45	<b>Coupling of Scales and Physics in Filtration and Separation Simulation</b> Dr. Ralf Kirsch, Fraunhofer ITWM
15:10	Coffee break (foyer)
<b>S3: MACHINE LEARNING FOR PROCESS ENGINEERING</b> Session Chair: Dr. Dietmar Hietel	
15:50	<b>Artificial Intelligence in Chemical Engineering: Past, Present and Future</b> Prof. Venkat Venkatasubramanian, PhD, Columbia University NY (USA)
16:40	<b>Model Development and Data Analyses for Industrial Thermal Separation Processes</b> Dr.-Ing. Thomas Gerlach, Bayer AG
17:05	<b>Machine Learning in Thermodynamics</b> Dr.-Ing. Fabian Jirasek, Prof. Dr.-Ing. Hans Hasse, TU Kaiserslautern
19:00	For speakers and external participants: Round table discussions and networking dinner

## PROGRAM – FRIDAY, OCTOBER 1

8:30	Arrival of participants, welcome coffee
<b>S4: MATERIAL FLOW</b> Session Chair: Dr. Raimund Wegener	
8:40	<b>Fluid Mechanic Shape Optimization with Phase Field Models</b> Prof. Dr. Michael Hinze, University of Koblenz-Landau, Campus Koblenz
9:30	<b>Prediction of Fouling in Continuous Polymerization Reactors by Means of Numerical Simulations and Engineering Correlations</b> Dr. Andreas Daiss, BASF SE
9:55	<b>Fluid Dynamical Design for Chemical Reactors</b> Dr. Christian Leithäuser, Fraunhofer ITWM
10:20	Coffee break (foyer)
<b>S5: SCHEDULING OF CONNECTED SYSTEMS</b> Session Chair: Dr. Konrad Steiner	
10:50	<b>Simultaneous Scheduling and Control of Dynamic Process Systems</b> Prof. Sandro Macchietto, PhD, Imperial College London (UK)
11:40	<b>Optimizing the Assets: The Lonza Way</b> Dr. Andreas Klein, Lonza AG
12:05	<b>Energy Efficient Drinking Water Supply</b> Dr. Dimitri Nowak, Fraunhofer ITWM
12:30	Lunch (foyer)
<b>S6: MSO FOR DYNAMIC PROCESSES II</b> Session Chair: PD Dr. Michael Bortz	
13:30	<b>Real-time Optimization: From First Principle Models to Machine Learning</b> Prof. Larry Biegler, PhD, Carnegie Mellon, Pittsburgh (USA)
14:20	<b>Bridging the Gap – Using Dynamics to Harmonize Simulation Activities Across all Disciplines</b> Dr. Jochen Steimel, Covestro AG
14:45	<b>Parameter Identification and Multicriteria Optimization of Bioprocesses</b> Dr.-Ing. Marco Baldan, Fraunhofer ITWM
15:10	Wrap up/closing
15:30	End of the workshop

### Invited speakers

- Prof. Larry Biegler, PhD, Carnegie Mellon, Pittsburgh (USA)
- Prof. Dr. Michael Hinze, University of Koblenz-Landau (D)
- Prof. Sandro Macchietto, PhD, Imperial College London (UK)
- Prof. Alexander Mitsos, PhD, RWTH Aachen (D)
- Prof. Dr. Hermann Nirschl, KIT (D)
- Prof. Venkat Venkatasubramanian, PhD, Columbia University NY (USA)