

Program



Tuesday, 2 September 2025

8:15–9:00	Registration		
8:50–9:00	Welcome remarks		
9:00–9:40	IS	Matt Knepley University at Buffalo, USA	Plasma Modeling with PETSc
9:40–10:00	CT	Saurav Samantaryay JGU Mainz	High order Asymptotic-Preserving penalized numerical schemes for the Euler-Poisson system in the quasineutral limit
10:00–10:20	CT	Valentin Churavy JGU Mainz	Scaling Julia up for HPC
10:20–10:50	Coffee break		
10:50–11:30	IS	Sam Stechmann University of Wisconsin-Madison, USA	Element learning: accelerating finite element-type methods via machine learning, and application to radiative transfer
11:30–12:10	IS	Patrick Rinke TU Munich	Machine-learning accelerated catalyst discovery and characterisation
12:10–13:40	Lunch		

12:10–13:40	Lunch, cont.		
13:40–14:20	IS	Dan Mendels Technion Israel Institute of Technology, Haifa	Machine Learning-Based Collective Variables and a Graph Neural Network Approach for Targeted Dynamics and Free Energy Manipulation in Molecular and Material Systems
14:20–14:40	CT	Simon Schneider JGU Mainz	Application of machine learning techniques to differential equations
14:40–15:00	CT	Ivan Utkin ETH Zurich & WSL Sion, Switzerland	Control of nonlinear bulk deformation and large shear strain on first-order phase transformation kinetics
15:00–15:20	CT	Andreas Schömer JGU Mainz	A hybrid multiscale method for the simulation of ring polymers
15:20–16:00	Coffee break		
16:00–18:00	Poster session & refreshments		

IS: Invited Speaker, CT: Contributed Talk

Topics:

Multiscale Methods

High Performance Computing & Machine Learning

Interdisciplinary Applications

Wednesday, 3 September 2025

9:00–9:40	IS	Tristan Bereau Heidelberg University	Free energies from score-based generative models
9:40–10:00	CT	Mattia Mazzucchelli University of Lausanne, Switzerland	Instability and equilibration of fluid-mineral systems under stress investigated through molecular dynamics
10:00–10:20	CT	Mahesh Yadav JGU Mainz	Biomolecular condensates with a Twist: From Assembly to Arrest
10:20–10:50	Coffee break		
10:50–11:30	IS	Rupert Klein Free University Berlin	Intensification of a tropical cyclone: Triple-deck theory for the control of convection
11:30–12:10	IS	Isabella Graf European Molecular Biology Laboratory, Heidelberg	Critical behavior in multicomponent mixtures with structured interactions: from tuning to function
12:10–13:40	Lunch		

12:10–13:40	Lunch, cont.		
13:40–14:20	IS	Ludovic Räss University of Lausanne, Switzerland	Using the Julia language to tackle portability and differentiable modelling at scale
14:20–14:40	CT	Nicolò Alagna University Medical Center, Mainz	Deep Learning Reaction Network (DLRN): a deep learning kinetic model analysis for time-resolved data
14:40–15:00	CT	Marios Andreou University of Wisconsin-Madison, USA	Assimilative Causal Inference
15:00–15:20	CT	Zhiqiang Zhang Max Planck Institute for Chemistry, Mainz	Kinetic modelling of non-equilibrium gas-particle partitioning in secondary organic aerosols: towards mass closure in atmospheric nanoparticle growth
15:20–16:00	Coffee break		
16:00–18:00	Poster session & refreshments		

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Topics:

- Multiscale Methods
- High Performance Computing & Machine Learning
- Uncertainty Quantification & Inverse Methods
- Interdisciplinary Applications

Thursday, 4 September 2025

9:00–9:40	IS	Gabriel Stoltz Ecole nationale des ponts et chaussées & Inria, Paris	Error estimates and variance reduction for nonequilibrium stochastic dynamics
9:40–10:00	CT	Michael te Vrugt JGU Mainz	The microscopic origin of thermodynamic irreversibility
10:00–10:20	CT	Enrique Muro JGU Mainz	Modeling the origin of Eukarya
10:20–10:50	Coffee break		
10:50–11:30	IS	Christian Kühn Technical University of Munich	Numerical Continuation for Random and Stochastic Differential Equations
11:30–11:50	CT	Ulrich Achatz Goethe University Frankfurt	Geophysical fluid dynamics on unresolved scales: Towards coupling gravity waves to turbulence, tracers and clouds
11:50–12:10	CT	Daniel Bäumer University of Vienna, Austria	PQG-DL-Ekman: a triple-deck boundary layer theory for large-scale atmospheric flow with moist process closures
12:10–13:40	Lunch		

12:10–13:40	Lunch, cont.		
13:40–14:20	IS	Franziska Glassmeier Max Planck Institute for Meteorology, Hamburg	A multiscale perspective on aerosol-cloud-climate cooling
14:20–14:40	CT	Franz Moritz Hey JGU Mainz	A cellular automaton approach to modeling secondary ice production
14:40–15:00	CT	Cornelis Schwenk JGU Mainz	The Role of Simulation Scale in Modeling Water Transport to the Upper Atmosphere
15:00–15:30	Coffee break		
15:30–15:50	CT	Arpit Babbar JGU Mainz	Single-Stage Time Integration Methods for Hyperbolic Partial Differential Equations
15:50–16:10	CT	Yuri Podladchikov University of Lausanne, Switzerland	Spontaneous strain and reactive fluid flow localization in space and time: interplay between continuum mechanics model formulations, numerical algorithms and HPC
16:10–16:30	CT	Hugo Dominguez JGU Mainz	Modelling volcanic eruptions from the volcano to the atmosphere
16:30–22:00	Conference dinner at Bonnheimer Hof		

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Topics:

- Stochastic Models
- Multiscale Methods
- Interdisciplinary Applications
- High Performance Computing & Machine Learning

Friday, 5 September 2025

9:00–9:40	IS	Mario Ohlberger University of Münster	Localized model reduction for multiscale problems with application in PDE constrained optimization
9:40–10:00	CT	Aravind Balan Indian Institute of Science, Bangalore, India	Optimal hp-adaptation for high-order discontinuous Galerkin methods for compressible flow simulations
10:00–10:20	CT	Stamen Dolaptchiev Goethe University Frankfurt	Modeling the Effects of Unresolved Gravity Waves on Ice Clouds
10:20–10:50	Coffee break		
10:50–11:30	IS	Lubomir Banas Bielefeld University, Bielefeld	Robust numerical approximation and adaptivity for the stochastic Cahn-Hilliard equation with singular noise
11:30–11:50	CT	Nelly Coulonges Free University Berlin	Toward consistent Particle-Continuum coupling with Fluctuating Hydrodynamics
11:50–12:10	CT	Simon Boisserée RWTH Aachen University, Aachen	Fluid flow channeling and mass transport with discontinuous porosity distribution
12:10–12:15	Closing remarks		
12:15–14:00	Lunch, optional		

IS: Invited Speaker, CT: Contributed Talk

Topics:

- Stochastic Models
- Multiscale Methods

List of Posters

Name	Affiliation	Title
Aellig Pascal	JGU Mainz	Small scale caldera collapse - A numerical study on central vent caldera-forming eruptions
Bali, Yogesh	JGU Mainz	Integrating Behavioral Survey Data into Epidemic Models: A Methodological Framework
Bartolome Garcia, Irene	JGU Mainz	Overshooting convection over southern Scandinavia: a modeling perspective
Bergner, Hannah	JGU Mainz	Ice clouds as nonlinear oscillators
Erenets, Ivan	MPI Chemistry	Kinetic Modeling and Optimization of Soot Gasification Processes
Filling, Jean Philip	JGU Mainz	Direct Molecular Polarizable Prediction with Local Frame GNNs on QM7-X
Frohlich, Simon	JGU Mainz	Realizing Quantitative Quasi-Particle Simulations of Skymion Dynamics in Arbitrary Potentials
Ibragimov, Iskander	JGU Mainz	High-Resolution Geodynamic Modeling of Volcanic Flank Instabilities Using HPC
Kang, Hyun Gu	MPI Chemistry	How can viscosity affect organic aerosol volatility derived from evaporation and thermal desorption measurements?
Knoth, Oswald	TROPOS Leibniz	Numerical weather forecasting with Julia
Labusch, Nikolaus	GU Frankfurt	Asymptotic and Machine Learning Parameterization of the Effect of Gravity Waves on Ice Clouds
Lee, Sangyun	JGU Mainz	Speed limits in terms of two entropy productions in a discrete-time Markov chain
Moutzouris, Dimitrios	JGU Mainz	Hamiltonian Monte Carlo applied in inverse petrological modeling
Pinto, Adrian	JGU Mainz	A coarse-grained model for SMC-mediated DNA loop extrusion
Popov, Anton	JGU Mainz	Scalable hybrid multigrid for staggered grid discretizations in geodynamics
Probst, Tristan	JGU Mainz	Numerical Simulations of Blood Flow in Realistic Human Arteries for the Assessment of Patient Specific Risk
Radecka, Maja	MPI Chemistry	A Kinetic Model of Multiphase Chemistry Integrating New Particle Formation and Size Distribution Dynamics in Secondary Organic Aerosol Formation (KM3C-NPF)
Rautela, Himani	Indian Inst. Tech. Roorkee	Breakdown of the Stokes–Einstein relation in Stillinger–Weber silicon
Schuler, Christian	JGU Mainz	Parameter Sensitivity Analysis of Plate Motion using the Adjoint Method and Automatic Differentiation
Sparmann, Tobias	JGU Mainz	A path integral approach to cloud modeling
Stroh, Annalena	JGU Mainz	Numerical modeling of simultaneous diffusion and mineral growth
Torregrosa Abellan, Antonio	JGU Mainz	Solutions of the population balance equation of cloud hydrometeors
Wörl, Ann-Christin	JGU Mainz	Reconstructing, Predicting and Understanding Cloud Structure Formations
Wroński, Michał	AGH Univ. Krakow	Numba-MPI & PyMPDATA: JIT-compilation and multi-threading for high performance computing in Python
Yang, Huan	MPI Chemistry	Molecular and nanoscale modeling in atmospheric aerosol processes
Zhang, Wenxiao	MPI Chemistry	Environmental and health impacts of urban residential energy switching in China
Zhang, Lijuan	MPI Chemistry	Aerosol–Cloud–Precipitation Interactions: Insights from Radar Observations and Model Simulations