# scales 2025

# Multiscale Modeling of Complex Systems

Mainz Institute of Multiscale Modeling

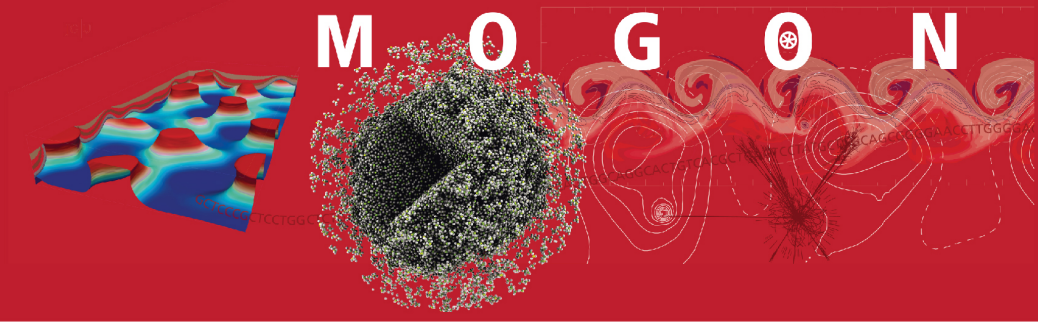
m3odel

**2nd SCALES Conference:**
**September 2 – 5**

**Workshop MPI/Open MP:**
**September 1**

**Johannes Gutenberg University, Mainz**

## PROGRAM & ABSTRACT VOLUME




MAX PLANCK INSTITUTE FOR POLYMER RESEARCH

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

MAX PLANCK INSTITUTE FOR CHEMISTRY

# Contents

# Welcome


## Mainz Institute of Multiscale Modeling

Spokespersons:
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# About

## M$^3$ODEL

Computational methods and data-driven modeling have become indispensable tools across the sciences. The highly interdisciplinary Mainz Institute of Multiscale Modeling brings together researchers from different areas in natural and life sciences with researchers in mathematics and computer science. Our research follows two main thrusts: developing multiscale models informed by simulation and experiment, and pushing the boundaries of computational methods.

**M$^3$ODEL** was established in July 2019 as one of the Top-level Research Areas funded through the Research Initiative of the State of Rhineland-Palatinate, and aims to facilitate and connect computational and modeling-oriented research across disciplines like atmospheric physics, biology, chemistry, geosciences, and physics combined with tools from mathematics and computer science. This consortium unites nearly 100 researchers – including professors, post-doctoral fellows, and students – from the Johannes Gutenberg University, the Max Planck Institute for Polymer Research, and the Max Planck Institute for Chemistry.

M$^3$ODEL continues a long tradition of interdisciplinary work that started with the platform Computational Science Mainz, supported by the excellent infrastructure available for high-performance computing with MOGON, the third-generation supercomputer at Johannes Gutenberg University. This allows scientists from many disciplines to achieve their competitive research objectives and advance interdisciplinary PhD projects that link information technology and/or numerical mathematics with the natural sciences.


**Johannes Gutenberg University Mainz**
Alte Mensa
55099 Mainz

**1–5 September 2025**

# SCALES

Multiscale methods are at the heart of modeling and understanding complex systems: Mathematical and algorithmic approaches to determine the behavior of complex systems at different scales, emerging from elementary principles. Methods are broad and interdisciplinary, ranging from bottom-up derivations of effective theories to top-down approaches of statistical machine learning.

The SCALES Conference on Multiscale Modeling of Complex Systems focuses on those methods on multiscale modeling and their interdisciplinary applications. SCALES 2025 is the 2$^{nd}$ of a series of biannual conferences held at the Johannes Gutenberg University in Mainz.

Sessions are organized around topics that emphasize on quantitative and predictive models and methods, including (but not limited to):

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

## Organizing Committee

| | | |
|---|---|---|
| Peter Spichtinger | Maria Lukáčová | Friederike Schmid |
| Michael Wand | Boris Kaus | Mariana Cosarinsky |

SCALES is made possible through the financial support of the Rhineland-Palatinate Research Initiative and the Carl Zeiss Foundation.

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Carl Zeiss
Stiftung

# Useful Information

**Talks** will be held at the **Atrium Max Auditorium** in the Alte Mensa on the campus of the Johannes Gutenberg University. It is situated on the ground floor of this traditional building, to the right of the foyer.

The **poster sessions** will be held on Tuesday and Wednesday in the **Linke Aula**, the lecture hall across the Atrium Max. Refreshments will be available.

**Coffee breaks** will be offered in the **Linke Aula**.

**Lunch** will be served daily in the Central Mensa, University Campus. Please, use the conference badge to pay. You can choose from a fixed menu (Theke 2) or a more varied option of warm meals and/or salad bar (Theke 1). If you don't use the badge, you will be asked to pay for the food with a Studicard, which you might not have and thus run into trouble. Please, don't forget the badge!

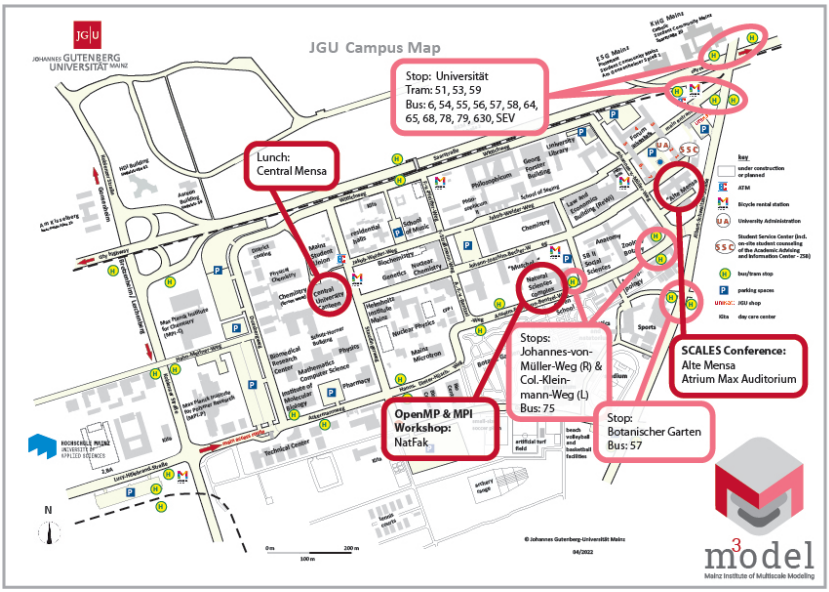
Wi-Fi is available on campus. You can access the network via eduroam.

# How to get there?

The Alte Mensa building is located on the eastern side of the campus and easy to reach by public transport from Mainz (stops Mainz Hauptbahnhof or Hauptbahnhof West):

- **Bus:** lines 6, 54, 55, 56, 57, 58, 64, 65, 68,, 78, 79, 630, SEV, stop Universität; line 75, stop Johannes-von-Müller-Weg; line 57, stop Botanischer Garten.
- **Tram:** lines 51, 53, 59, stop Universität.

Please, make sure to check for possible route or schedule changes, especially of the tram lines, due to construction sites in the city center.



# Social Event

The conference dinner will take place on the evening of Thursday September 4$^{th}$ at the restaurant **Bonnheimer Hof** in Hackenheim.

We have arranged transportation. The meeting point is outside the Alte Mensa building at 16:40.

# Program

## Monday, 1 September 2025

Pre-conference Workshop **MPI/OpenMP**

**Lecturer:** Dr. Rolf Rabenseifner – HLRS High-Performance Computing Center Stuttgart

**Time:** 9:00 – 17:00

**Place:** Senatssaal 7$^{th}$ floor, NatFak Building, J.-J.-Becher-Weg 21 D-55128 Mainz

The goal of this course is to give people with some programming experience an introduction to the MPI and OpenMP parallel programming models. Hands-on exercises will allow participants to immediately test and understand the Message Passing Interface (MPI) constructs and OpenMP's shared memory directives. Please, bring your own computer. We will provide lunch and refreshments.

# Tuesday, 2 September 2025

| | | | |
|---|---|---|---|
| 8:15–9:00 | **Registration** | | |
| 8:50–9:00 | **Welcome remarks** | | |
| 9:00–9:40 | IS | **Matt Knepley**<br>University at Buffalo, USA | Plasma Modeling with PETSc |
| 9:40–10:00 | CT | **Saurav Samantaray**<br>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**<br>JGU Mainz | Scaling Julia up for HPC |
| 10:20–10:50 | **Coffee break** | | |
| 10:50–11:30 | IS | **Sam Stechmann**<br>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**<br>Technical University of Munich | Machine-learning accelerated catalyst discovery and characterisation |
| 12:10–13:40 | **Lunch** | | |

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|---|---|---|---|
| 12:10–13:40 | **Lunch, cont.** | | |
| 13:40–14:20 | IS | **Dan Mendels**<br>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**<br>JGU Mainz | Application of machine learning techniques to differential equations |
| 14:40–15:00 | CT | **Ivan Utkin**<br>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**<br>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**<br>Heidelberg University | Free energies from score-based generative models |
| 9:40–10:00 | CT | **Mattia Mazzucchelli**<br>University of Lausanne, Switzerland | Instability and equilibration of fluid-mineral systems under stress investigated through molecular dynamics |
| 10:00–10:20 | CT | **Mahesh Yadav**<br>JGU Mainz | Biomolecular condensates with a Twist: From Assembly to Arrest |
| 10:20–10:50 | **Coffee break** | | |
| 10:50–11:30 | IS | **Rupert Klein**<br>Free University Berlin | Intensification of a tropical cyclone: Triple-deck theory for the control of convection |
| 11:30–12:10 | IS | **Isabella Graf**<br>European Molecular Biology Laboratory, Heidelberg | Critical behavior in multicomponent mixtures with structured interactions: from tuning to function |
| 12:10–13:40 | **Lunch** | | |

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|---|---|---|---|
| 12:10–13:40 | **Lunch, cont.** | | |
| 13:40–14:20 | IS | **Ludovic Räss**<br>University of Lausanne, Switzerland | Using the Julia language to tackle portability and differentiable modelling at scale |
| 14:20–14:40 | CT | **Nicolò Alagna**<br>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**<br>University of Wisconsin-Madison, USA | Assimilative Causal Inference |
| 15:00–15:20 | CT | **Zhiqiang Zhang**<br>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** | | |

IS: Invited Speaker, CT: Contributed Talk

Topics:

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

# Thursday, 4 September 2025

| | | | |
|---|---|---|---|
| 9:00–9:40 | IS | **Gabriel Stoltz**<br>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**<br>JGU Mainz | The microscopic origin of thermodynamic irreversibility |
| 10:00–10:20 | CT | **Enrique Muro**<br>JGU Mainz | Modeling the origin of Eukarya |
| 10:20–10:50 | **Coffee break** | | |
| 10:50–11:30 | IS | **Christian Kühn**<br>Technical University of Munich | Numerical Continuation for Random and Stochastic Differential Equations |
| 11:30–11:50 | CT | **Ulrich Achatz**<br>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**<br>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** | | |

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|---|---|---|---|
| 12:10–13:40 | **Lunch, cont.** | | |
| 13:40–14:20 | IS | **Franziska Glassmeier**<br>Max Planck Institute for Meteorology, Hamburg | A multiscale perspective on aerosol-cloud-climate cooling |
| 14:20–14:40 | CT | **Franz Moritz Hey**<br>JGU Mainz | A cellular automaton approach to modeling secondary ice production |
| 14:40–15:00 | CT | **Cornelis Schwenk**<br>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**<br>JGU Mainz | Single-Stage Time Integration Methods for Hyperbolic Partial Differential Equations |
| 15:50–16:10 | CT | **Yuri Podladchikov**<br>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**<br>JGU Mainz | Modelling volcanic eruptions from the volcano to the atmosphere |
| 16:30–22:00 | **Conference dinner at Bonnheimer Hof** | | |

IS: Invited Speaker, CT: Contributed Talk

Topics:

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

# Friday, 5 September 2025

| | | | |
|---|---|---|---|
| 9:00–9:40 | IS | **Mario Ohlberger**<br>University of Münster | Localized model reduction for multiscale problems with application in PDE constrained optimization |
| 9:40–10:00 | CT | **Aravind Balan**<br>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**<br>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**<br>Bielefeld University, Bielefeld | Robust numerical approximation and adaptivity for the stochastic Cahn-Hilliard equation with singular noise |
| 11:30–11:50 | CT | **Nelly Coulonges**<br>Free University Berlin | Toward consistent Particle-Continuum coupling with Fluctuating Hydrodynamics |
| 11:50–12:10 | CT | **Simon Boisserée**<br>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

# Oral Presentations

## Geophysical fluid dynamics on unresolved scales: Towards coupling gravity waves to turbulence, tracers and clouds

*U. Achatz*[1], *T. Banerjee*[1], *S. Dolaptchiev*[1], *I. Knop*[1], *A. Kosareva*[1]

[1]Institute for Atmospheric and Environmental Sciences, Goethe University Frankfurt, Frankfurt am Main, Germany

Topic: Multiscale Methods **CT**

Atmosphere and ocean sciences are faced by substantial efforts to develop climate models resolving horizontal motions on the km scale. This will provide dynamically consistent data that can be used for detailed studies of a wealth of processes. Geophysical Fluid Dynamics (GFD) with all its mathematical tools will be an essential element in these developments. Without it we would be left with admiring the shear complexity we are confronted with and describing selective details that catch our interest, while not being able to understand the grand picture in a conceptually satisfying way. Mathematical theory should accompany both idealized and local process studies and global-scale investigations to provide the understanding we need for the competence that our advice to policy makers should rest on.

A line of research in this context addresses the dynamics of atmospheric gravity waves. They are known to both have leading-order global-scale effects on the atmospheric circulation and influence the distribution of water vapor, ice, and other substances of relevance for the climate impact of solar radiation. At the same time, they are both influenced by and affecting various other small-scale components of the atmosphere, e.g. turbulence and clouds. Such aspects are being studied using a Lagrangian approach to parameterizing gravity waves by predicting their three-dimensional propagation and formulating their mean-flow impact. The theory and numerical approach of this Multi-Scale Gravity-Wave Model MS-GWaM [1,2,3] is continuously being developed and tested in idealized simulations, using an in-house flow solver. MS-GWaM has also been implemented into the climate model ICON to investigate global-scale gravity-wave effects.

Recent developments to be reported here are the incorporation of gravity-wave effects on tracer transport and mixing, and on ice clouds. Multi-scale asymptotic theory has been used to formulate a gravity-wave Stokes drift, predominant in the presence of rotation, and a next-order coupling that might be more relevant in the tropics. The incorporation of these effects into MS-GWaM is validated against wave resolving simulations. First steps towards a theory coupling gravity waves and turbulence will also be presented. This is not only to lead to an improved description of gravity-wave breaking but it also introduces a corresponding turbulence source that potentially has important effects on tracer mixing, as demonstrated within ICON. Finally, the effect of gravity waves on ice clouds shall be touched, where asymptotic theory has been used to formulate the effect on ice-cloud formation without having to resolve this process in time. First steps in ICON indicate a significant effect of convectively generated gravity waves on cirrus in the tropical tropopause layer.

References:
[1] Achatz U., Kim Y.-H., Voelker G.S. Multi-scale dynamics of the interaction betweenwaves and mean flows: From nonlinear WKB theory to gravity-wave parameterizations in weather and climate models. J. Math. Phys. 64, 111101 (2023) doi: 10.1063/5.0165180
[2] Voelker G.S., Bölöni G., Kim Y., Zängl G., Achatz U. MS-GWaM: A Three-Dimensional Transient Gravity Wave Parametrization for Atmospheric Models. J. Atmos. Sci. 81, 1181-1200 (2024) doi:10.1175/JAS-D-23-0153.1.
[3] Kim Y.-H., Voelker G.S., Bölöni G., Zängl G., Achatz U. Crucial role of obliquely propagating gravity waves in the quasi-biennial oscillation dynamics, Atmos. Chem. Phys. 24, 3297-3308 (2024) doi:10.5194/acp-24-3297-2024

## Deep Learning Reaction Network (DLRN): a deep learning kinetic model analysis for time-resolved data

*N. Alagna*[1], *B. Dúzs*[2], *V. Dietrich*[1], *A.T. Younesi*[3], *L. Lehmann*[2], *R. Ulbricht*[3], *H. Köppl*[4], *A. Walther*[2], *S. Gerber*[1]

[1]Institute of Human Genetics, University Medical Center, Mainz, Germany; [2]Dept. of Chemistry, Johannes Gutenberg University, Mainz, Germany; [3]MPI for Polymer Research, Mainz; [4]Centre for Synthetic Biology, Technical University Darmstadt, Germany

Topic: Uncertainty Quantification & Inverse Methods, Multiscale Methods

**CT**

Model-based analysis is essential for extracting information about chemical reaction kinetics in full detail from time-resolved data sets. Such analysis combines experimental hypotheses with mathematical and physical models related to the system, which can provide a concise description of complex dynamics and extrapolate kinetic model parameters, such as kinetic pathways, time constants, and species amplitudes. However, the process leading to the final kinetic model requires several intermediate steps in which different assumptions and models are tested and combined multiple experiments. This approach requires considerable experience in modeling and data comprehension, as poor decisions at any stage of time-resolved data analysis can lead to an incorrect or incomplete kinetic model, resulting in inaccurate results. Here, we present DLRN (Deep Learning Reaction Network), a deep neural network architecture created to combine GTA and ML methods. DLRN can disentangle all the kinetic information from a 2D time-resolved data set, giving the most probable kinetic model, related time constants for each pathway, and a maximum of four SAS for one time scale. Moreover, DLRN can analyze systems in which the initial state is a non-emitting dark state. DLRN was also tested to analyze 2D data at multiple time scales, achieving good performance and the ability to identify complex kinetic models that have a higher number of variables (but not for each timescale) than those used during training. DLRN performed well in the analysis of both time-resolved spectra and agarose gel electropherograms. Moreover, DLRN was also tested to analyze the kinetic reaction of nitrogen-vacancy (NV) centers and DNA strand displacement (DSD) measured using experimental techniques (photoluminescence -PI- and transient absorption -TA- for NV). Results show that the neural network was able to extract the correct expected kinetic models, including their variables, for the experimental systems here analyzed.

References:
[1] Alagna N. et al. Deep Learning Reaction Framework (DLRN) for kinetic modeling of time-resolved data. Commun. Chem. 8, 153 (2025)

## Assimilative Causal Inference

*M. Andreou*[1], *N. Chen*[1], *E. Bollt*[2]

[1]Department of Mathematics, University of Wisconsin-Madison, Madison, WI, USA; [2]Department of Mathematics and Department of Electrical and Computer Engineering, Clarkson University, Potsdam, NY, USA

Topic: Uncertainty Quantification & Inverse Methods, Stochastic Models

CT

Causal inference is fundamental across scientific disciplines, yet state-of-the-art methods often struggle to capture instantaneous, time-evolving causal relationships in complex, high-dimensional systems. This work introduces assimilative causal inference (ACI), a paradigm-shifting framework that leverages Bayesian data assimilation to trace causes backward from observed effects. ACI formulates and solves an implicit Bayesian inverse problem to assess uncertainty reduction in the estimated state from incorporating future information about effect variables, rather than quantifying forward influence. It uniquely identifies dynamic causal interactions without requiring observations of candidate causes, accommodates short datasets, and scales efficiently to high dimensions. Crucially, it provides online tracking of causal roles, which may reverse intermittently, and facilitates the development of a mathematically rigorous criterion for the temporal causal influence range (CIR) associated with each causal link. The ACI-based CIR metric is objectively defined, avoiding ad hoc or subjective empirical thresholds, and admits both forward- and backward-in-time formulations to quantify how far effects propagate and to attribute them to past causes, respectively. The effectiveness of ACI is demonstrated on complex nonlinear dynamical systems showcasing intermittency and extreme events. ACI opens new avenues for studying complex systems, where transient causal structures are critical. [1]

References:

[1] Andreou M., Chen N., Bollt E. Assimilative Causal Inference, arXiv. (2025) doi:10.48550/arXiv.2505.14825

## Single-Stage Time Integration Methods for Hyperbolic Partial Differential Equations

*A. Babbar*[1,2], *H. Ranocha*[1,2], *Q. Chen*[3]

[1]Institute of Mathematics, Johannes Gutenberg University, Mainz, Germany; [2]Mainz Institute of Multiscale Modeling, Johannes Gutenberg University, Mainz, Germany; [3]Department of Mathematics, Ohio State University, Columbus, USA

Topic: HPC & Machine Learning; Multiscale Methods **CT**

Hyperbolic partial differential equations (PDEs) arise in a wide range of practical applications, including computational fluid dynamics (CFD), astrophysics, and weather modeling. These applications are often complex and computationally demanding, making the development of efficient numerical methods a critical area of research. High-order methods, which improve accuracy without excessively refining the computational mesh, are known to be particularly useful in this direction.

Traditionally, high-order methods for hyperbolic PDEs combine high-order spatial discretization with multi-stage Runge-Kutta schemes for time integration. This talk explores an alternative approach: single-stage time integration methods. These methods reduce the amount of data exchange required during computation, making them particularly well-suited for modern high-performance computing (HPC) architectures.

The presentation will begin with a review of some single-stage time integration methods from the literature. The main focus will be on recent developments in compact Runge-Kutta methods, as introduced in [1]. We will discuss extensions of these methods to non-conservative hyperbolic PDEs, treatment of source terms with distinct time scales from advection, and strategies to enforce physical constraints, such as positivity of density and pressure.

References:
[1] Chen Q., Sun Z., Xing Y. The runge-kutta discontinuous galerkin method with compact stencils for hyperbolic conservation laws. SIAM Journal on Scientific Computing (2024)

## Optimal hp-adaptation for high-order discontinuous Galerkin methods for compressible flow simulations

*A. Balan*[1], *D. Kain*[1], *P. Tank*[1]

[1]Department of Aerospace Engineering, Indian Institute of Science, Bangalore, India

Topic: Multiscale Methods **CT**

High-order discontinuous Galerkin (DG) methods are suitable for hp-adaptation, where both the mesh element size (h) and the solution polynomial degree (p) can be adapted on the domain to efficiently resolve the flow features. For mesh adaptation, metric-based mesh adaptation offers a convenient way to generate optimal anisotropic adapted meshes. The talk focuses on metric-based hp-adaptation for DG methods. A high-order interpolation error estimate suitable for DG methods is used to construct the metric field and the polynomial degree distribution in the domain. The metric field is used to generate a quasi-structured quad dominant mesh that can efficiently resolve boundary layers and shocks arising in compressible flows. Eigen-vector information from the metric-field is used to generate the quasi-structured triangular meshes, which are then combined in an optimal manner to get the quasi-structured quad meshes. The methodology is verified with various test cases. For a scalar convection diffusion test case, hp-adaptation is shown to give more accurate results than pure h-adaptation and uniform refinement for a given number of degrees of freedom (DoF). For a subsonic viscous case, the separation regions are also better captured with hp-adaptation.

References:

[1] Balan A. et al. A review and comparison of error estimators for anisotropic mesh adaptation for compressible flows. Computers and Fluids (2022)

## Robust numerical approximation and adaptivity for the stochastic Cahn-Hilliard equation with singular noise

*L. Banas*[1]

[1]Department of Mathematics, Bielefeld University, Bielefeld, Germany

Topic: Stochastic Models **IS**

We discuss a posteriori error estimates for a fully discrete finite element approximation of the stochastic Cahn-Hilliard equation with singular noise. To deal with the low spatial regularity of the noise we consider a regularized problem with suitable approximation of the space-time white noise. We derive an a posteriori error bound for the regularized problem by a splitting of the equation into a linear stochastic partial differential equation and a nonlinear random partial differential equation. The estimate for the discretization of the original problem is then obtained by considering suitable probability subsets with high probability. The resulting a posteriori estimate is computable and robust with respect to the interfacial width parameter as well as the noise intensity. We illustrate the theoretical result by numerical simulations.

The talk is based on a joint work with Christian Vieth and Jean Daniel Mukam.

Lubomir Banas received his PhD in mathematics from Ghent University in 2005, following his undergraduate studies at Comenius University Bratislava. After a two-year postdoctoral fellowship at Imperial College London, he served as a lecturer at Heriot-Watt University in Edinburgh from 2007 to 2013. He has been Professor of Mathematics at Bielefeld University since 2013. His research focuses on numerical analysis, scientific computing, and mathematical modeling, with a particular emphasis on nonlinear (stochastic) partial differential equations (PDEs). He aims to develop, analyze, and implement efficient and reliable numerical schemes for these problems. His work also extends to the numerical approximation of PDE-constrained optimal control problems and probabilistic approximation methods for Hamilton-Jacobi-Bellman equations which arise in differential games.

## PQG-DL-Ekman: a triple-deck boundary layer theory for large-scale atmospheric flow with moist process closures

*D. Bäumer*[1], *R. Klein*[2]

[1]Research platform MMM, Faculty of Mathematics, University of Vienna, Vienna, Austria; [2]Department of Mathematics and Computer Sciences, Free University Berlin, Germany

Topic: Multiscale Methods, Interdisciplinary Applications **CT**

Reduced mathematical models for atmospheric dynamics at various scales have a long and rich history. However, versions of such models that explicitly incorporate moisture and phase changes have been developed only fairly recently. This work merges one of said modeling innovations, namely Smith and Stechmann's *precipitating quasigeostrophic* (PQG) model family, with a triple-deck boundary layer theory due to Klein et al. that extends the classical QG-Ekman theory by an intermediate *diabatic layer* (DL). A detailed analysis of the Clausius-Clapeyron relation and Kessler-type bulk microphysics closures is included in the systematic derivation of the resulting PQG-DL-Ekman theory. Furthermore, to illustrate some of the model's properties, explicit axisymmetric solutions of the precipitating diabatic layer equations are derived and combined with numerical sample solutions for the bulk flow. [1]

References:
[1] Bäumer D., Klein R. PQG-DL-Ekman: a triple-deck boundary layer theory for large-scale atmospheric flow with moist process closures (submitted)

## Free energies from score-based generative models

*T. Bereau* [1]

[1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Topic: Multiscale Methods, HPC & Machine Learning **IS**

Accurate free-energy estimation often requires many intermediate states or suffers from slow convergence. We present two score-based frameworks that dramatically reduce sampling costs. The first project, neural Thermodynamic Integration (Neural TI), encodes a continuous, time-dependent Hamiltonian between two states. Optimized via score matching, the energy-based model learns log-density gradients across all intermediates, enabling free-energy differences from a single simulation. Benchmarks, including Lennard-Jones fluids and water/methane solvation, show high accuracy with only a single reference simulation [1,2]. The second project, Fokker-Planck Score Learning, tackles non-equilibrium pulling when the collective variable corresponds to the simulation box. Mapping periodic boundary simulations onto a Brownian particle in a periodic potential allows us to derive an analytic Fokker-Planck score encoding free-energy gradients. Training on brief non-equilibrium trajectories lets us reconstruct the potential of mean force efficiently, outperforming umbrella sampling by up to tenfold in small-molecule membrane permeation [3].

References:
[1] Máté B., Fleuret F., Bereau T. J Phys Chem Lett 15(45), 11395-11404 (2024)
[2] Máté B., Fleuret F., Bereau T. J Chem Phys 162(12) (2025)
[3] Nagel D., Bereau T. arXiv:2506.15653 (2025)

**About:**

Tristan Bereau is a computational physicist working at the interface between multiscale modeling and machine learning for soft matter and biomolecules. He earned a Ph.D. in Physics at Carnegie Mellon University in 2011. After a postdoc at the University of Basel, he led an Emmy Noether research group at the Max Planck Institute for Polymer Research. He then moved to the University of Amsterdam as an assistant professor in chemistry and computer science, followed by a role in Industry. Tristan serves on the editorial boards of the journals Machine Learning: Science & Technnology and Computational Science and Engineering. He is currently a professor at the Institute for Theoretical Physics at the University of Heidelberg. His research focuses on the development and application of multiscale molecular simulations methods for soft-condensed-matter materials. He is particularly invested in using multiscale modeling to explore chemical compound space.

## Fluid flow channeling and mass transport with discontinuous porosity distribution

*M. Bachmayr*[1], *S. Boisserée*[1], *E. Moulas*[2]

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Topic: Multiscale Methods, Interdisciplinary Applications **CT**

The flow of fluids within porous rocks is an important process with numerous applications in Earth sciences. Modeling the compaction-driven fluid flow requires the solution of coupled nonlinear partial differential equations that account for the fluid flow and the solid deformation within the porous medium. Despite the nonlinear relation of porosity and permeability that is commonly encountered, natural data show evidence of channelized fluid flow in rocks that have an overall layered structure. Layers of different rock types routinely have discontinuous hydraulic and mechanical properties. We present numerical results [1] obtained by a novel space-time method [2] based on a fixed-point scheme inspired by the mathematical analysis [3], combined with a space-time least-squares formulation. This approach can handle discontinuous initial porosity (and hence permeability) distributions. It furthermore exhibits optimal convergence independently of the discontinuities, while standard approximations, as e.g. finite differences, tend to show lower order convergence in discontinuous regimes. The space-time method enables a straightforward coupling to models of mass transport for trace elements. Our results show the influence of different kinds of layering in the development of fluid-rich channels and mass transport [1].

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## Scaling Julia up for HPC

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[1]Institute of Mathematics, Johannes Gutenberg University, Mainz, Germany; [2]High-Performance Scientific Computing, Centre for Advanced Analytics and Predictive Sciences, University of Augsburg, Germany

Topic: HPC & Machine Learning, Uncertainty Quantification & Inverse Methods

CT

Julia is a modern programming language, tailored towards scientific computing. To address scientific questions of today and tomorrow scientists need to perform computations at a large scale on compute architectures that have a diverse mix of hardware. This talk will cover learnings from scaling Julia up, enabling usage that ranges from laptops to supercomputers, with a wide variety of GPU hardware support. A particular challenge in the age of increasingly diverse compute architectures is to provide users a consistent and performant compute environment.

## Toward consistent Particle-Continuum coupling with Fluctuating Hydrodynamics

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Topic: Multiscale Methods, Interdisciplinary Applications **CT**

Understanding how to accurately couple particle-based systems with continuum scale solvers is critical for modeling multiscale phenomena in soft matter and biological systems. In particular, scenarios involving nanoscale or molecular processes embedded in a larger fluid domain—such as the electrochemical surface processes and largescale transport around "artificial leafs"[1] that turn sunlight into the chemically bound energy of suitable substances, or thermophoretic microswimmers [2]. In previous work [1], a hybrid simulation framework was developed in which a particle-based open system (AdResS) is coupled with a Fluctuating Hydrodynamics (FHD) solver, enabling the modeling of systems such as lipid membranes immersed in thermal reservoirs. This framework is grounded in the Liouville hierarchy for open systems and allows for local thermodynamic parameters (e.g., temperature) to be controlled via the continuum solver. Conventional FHD models represent thermal fluctuations—stemming from microscopic-scale irregular dynamics—as spatially uncorrelated noise. However, we argue that the fluxes at the boundaries of a control volume, in both particle-based and continuum frameworks, should exhibit spatial correlations that are essential to capture for a consistent coupling. Our objective is to characterize these fluctuations by analyzing their correlation structure, which will ultimately inform the formulation of coupling conditions and support the study of the Liouville hierarchy in an intermediate scaling regime relevant for FHD. Specifically, we aim to identify a mesoscale: a regime small enough for thermal fluctuations to significantly influence the dynamics, yet large enough for those fluctuations to be effectively described by a Markovian process with Gaussian noise. Our approach is to use molecular dynamics simulations to obtain statistical information about the mass, momentum and energy fluxes across the boundaries of a control volume and to provide an analysis of the correlation structure by observing the spread of a perturbation in the fluid. By identifying the relevant correlation structures at the mesoscale, our results pave the way for more physically accurate hybrid models that bridge microscopic simulations and continuum descriptions. This work contributes to the theoretical foundations for multiscale modeling in systems where thermal fluctuations are non-negligible, with potential applications in soft matter, nanofluidics, and biological systems.

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## Modeling the Effects of Unresolved Gravity Waves on Ice Clouds

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Topic: Multiscale Methods **CT**

Atmospheric gravity waves (GWs) play a signifcant role in the formation and evolution of cirrus clouds. However, even kilometer-scale global numerical weather prediction and climate models can only partially resolve the GW spectrum, necessitating the use of GW parameterizations to account for the missing variability. These parameterizations are often only crudely integrated with ice physics parameterizations, leading to substantial uncertainties regarding the radiative impact of ice clouds due to unresolved dynamics. In this presentation, we will introduce an novel approach to integrate the effects of GWs on ice physics within transient GW parameterizations, such as the Multiscale Gravity Wave Model (MS-GWaM) [1]. We begin by performing an asymptotic analysis of the equations governing GW dynamics and ice physics, allowing us to identify the dominant interaction mechanisms. Applying matched asymptotic techniques, we construct prototype parameterization for the homogeneous nucleation of ice crystals caused by rapid fluctuations, such as those generated by GWs [2]. Subsequently, we couple this parameterization to MS-GWaM and validate its performance by comparing the results of wave- and nucleation-parameterized simulations with those of wave and nucleation-resolving simulations in idealized setups. Finally, we present the application of our approach to realistic global atmospheric simulations conducted within the ICON/MS-GWaM framework.

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## Modelling volcanic eruptions from the volcano to the atmosphere

*H. Dominguez*[1], *B.J.P. Kaus*[1,2], *H. Ranocha*[2,3], *E. Moulas*[1,2], *I. Utkin*[4,5]

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Topic: Interdisciplinary Applications CT

Volcanic eruptions are among the most destructive natural hazards, with the potential to disrupt lives and socio-economic activities on local to global scales. Physically, they are complex, multiphase phenomena that involve tightly coupled processes between ascending magma, exsolved volcanic gases, host rock deformation, and atmospheric dynamics. So far, most numerical models have focused on either the material ejected during the eruption and its interplay with the atmosphere or on the rock deformation of the volcano itself during eruption. This is because modelling the interplay between solid and air at the same time is complex and involves important differences in timescales and material properties. This study presents the preliminary results of a 2D numerical model that couples wave propagation in the atmosphere and elastic deformation in the surrounding host rock during a volcanic eruption. The model employs a unified formulation and discretisation approach to solve the conservative form of the mass and momentum conservation equations on a staggered grid using a finite volume method. The results demonstrate that this formulation captures both the transmission of acoustic waves from the atmosphere into the host rock as elastic waves and the reverse process. These results represent a first step towards more coupled models of volcanic systems, offering new insights into how atmospheric and subsurface processes interact during explosive events.

## A multiscale perspective on aerosol-cloud-climate cooling

*F. Glassmeier*[1]

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Topic: Multiscale Methods **IS**

The complexity of clouds not only puzzles the casual observer but also challenges our understanding of Earth's climate and climate change. The processes that make clouds so hard to capture range from the formation of cloud droplets on aerosol particles to the mesoscale self-organization of cloud fields into patterns to the change of cloud type with large-scale conditions. The response of such multiscale cloud systems to aerosol perturbations tends to cool the planet but remains the most uncertain anthropogenic forcing of the climate system. Cooling and uncertainty are dominated by stratocumulus cloud decks, which exhibit bi-stable mesoscale behavior between a reflective, high-cloud-fraction state, and a less reflective, low-cloud-fraction state.

I will model aerosol-stratocumulus interactions as a data-driven and physics-informed stochastic dynamical system with time-dependent parameters. This description encapsulates the scales of cloud formation, mesoscale self-organization into patterns, and large-scale conditions in stochastic fluctuations, deterministic evolution, and parameters, respectively. The sparsity of available data is augmented by physical process understanding.

This 3-scale effective model allows us to discuss the non-linear response of stratocumulus to aerosol perturbations. We find that mesoscale aerosol perturbations, as e.g. emitted by industrial centers, have the strongest impact on the transition between patterns of high- and low-cloud fraction. Similarly, we observe mesoscale memory of short-lived perturbations that mimic ship exhaust. Overall, our results highlight that the mesoscale needs to be considered by climate models if we are to constrain the anthropogenic aerosol forcing of the climate system.

**About:**
Franziska Glassmeier leads a Lise Meitner Group at the Max Planck Institute for Meteorology in Hamburg and is an Associate Professor at Delft University of Technology. She studied Physics at the University of Göttingen and earned her PhD from ETH Zurich in 2016, followed by positions at NOAA and Wageningen University. Franziska's research is motivated by the complexity of clouds across scales and has been awarded prestigious funding, most recently an ERC Starting Grant.

## Critical behavior in multicomponent mixtures with structured interactions: from tuning to function

*I. Graf*[1]

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Topic: Multiscale Methods **IS**

It is increasingly recognized that the phase behavior of mixtures with many components plays an important role in biology, both for the formation of membrane-less compartments in the cytosol as well as for the functional behavior of plasma membranes. Indeed, cell-derived plasma membranes, composed of thousands of components, are tuned close to a miscibility critical point and actively adapt their membrane composition to stay near this critical point when grown at different temperatures. But how can these systems find the critical manifold in the very high-dimensional parameter space of membrane composition? And what (coarse-grained) parameters even determine critical behavior? To address this question, we have developed a theoretical framework for mixtures made up from a large number of components that interact through a smaller number of features in terms of a structured interaction matrix. I will show that thermodynamic stability and critical behavior only depend on the distribution of the components in the lower-dimensional space of features, and that a simple feedback motif inspired by previous work of ours on sensory systems can robustly keep the mixture close to the critical point. Finally, I will discuss potential benefits of critical membrane behavior for function.

**About:**
Isabella Graf graduated at Ludwig Maximilian University of Munich. After a postdoctoral stay at Yale University, she obtained a group leader position at EMBL Heidelberg in 2024. In her research, she studies how living systems manage to stay resilient while adapting to constantly changing environments. Her work focuses on uncovering the principles that allow life to be both flexible and stable at the same time and to understand the role of phase transitions and critical points in shaping biological behavior. To do this, she combines approaches from physics, mathematics, and information theory, and collaborates closely with experimental scientists.

## A cellular automaton approach to modeling secondary ice production

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[1]Institute of Atmospheric Physics, Johannes Gutenberg University, Mainz, Germany

Topic: Stochastic Models, Interdisciplinary Applications **CT**

Studies have shown that there exist far more ice-particles in clouds than ice-nucleating particles (INP). This means that in addition to primary ice production (the freezing of supercooled water directly on INP) there has to be an additional mechanism at play: secondary ice production which does not need INP to produce new ice particles. [1] Our goal is to develop a model which can reproduce the physical process of secondary ice productions, as, e.g., breakup and thus also ice particle-size distributions measured in clouds. This model approach should help to quantify the underlying processes of secondary ice production. For this goal we will treat ice formation as a morphological problem, asking how we can replicate the observed shapes and structures in the simplest way. Cellular Automata are very well suited for this purpose because of their ability to produce complex patterns with simple underlying rules. The model will therefore be constructed in the form of a cellular automaton with several rules allowing for connected growth and decay cycles of ice-crystals.

References:
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# Intensification of a tropical cyclone: Triple-deck theory for the control of convection

*R. Klein* [1]

[1]Department of Mathematics and Computer Sciences, Free University Berlin, Germany

Topic: Multiscale Methods **IS**

Focusing on upright axisymmetric vortices, this work demonstrates that an asymptotic triple-deck expansion for vortices in gradient wind balance enables the theoretical explanation of several important observational features of tropical storms and incipient hurricanes and typhoons. For instance, super-gradient winds are naturally found in the friction layer (FL), and the newly introduced intermediate layer hosts the lifting condensation level (LCL), the level of free convection (LFC) and, under suitable conditions, a layer of convection inhibition (CIN). Due to its significance for the onset of convective processes that feed back into the primary circulation, this intermediate layer is labeled "convection controlling layer" (CCL). It is revealed how, driven by multi-scale convection, angular momentum transport between the three layers induces vortex intensification.

**About:**

Rupert Klein holds a doctorate degree (1988) and habilitation (1995) in Mechanical Engineering from RWTH Aachen University with specialization in "Nonstationary Mechanics". Following his rising interest in environmental science, he accepted an offer to take up a professorship on "Safety Technology" at Bergische Universität Wuppertal in 1995. Two years later, he received a two-legged appointment by Freie Universität Berlin (FUB) and the Potsdam-Institut for Climate Impact Research (PIK) to become the head of the "Data & Computation" Department at PIK (1997-2007) and to establish a research group on "Scientific Computing/Modelling and Simulation of Global Environmental Systems" within the Mathematics & Informatics Department of FUB. His research covers topics of theoretical and computational fluid dynamics in a broad sense, with applications to atmospheric flows, vortex dynamics, and combustion. [Picture courtesy of the Oberwolfach Photo Collection https://opc.mfo.de/]

## Plasma Modeling with PETSc

*M.G. Knepley*[1]

[1]Department of Computer Science and Engineering, University at Buffalo, Buffalo, NY, USA

Topic: Interdisciplinary Applications, Multiscale Methods **IS**

We present a framework for simulating the Vlasov-Poisson-Landau equations for plasma physics using a Particle-In-Cell (PIC) discretization with finite elements on the background grid. We use a novel conservative projection scheme to move between discretizations, and construct moment equations. The timestepping is likewise constructed to preserve the conservation and stability properties of the spatial discretization. These software modules are intended to be composable, and easily applied to other phenomenology.

**About:**

Matthew G. Knepley is a Professor in the Computer Science and Engineering Department of the University at Buffalo. He received his B.S. in Physics from Case Western Reserve University in 1994, an M.S. in Computer Science from the University of Minnesota in 1996, and a Ph.D. in Computer Science from Purdue University in 2000. He was a Research Scientist at Akamai Technologies in 2000–2001 in the Distributed Data Collection and Data Analysis groups. Afterwards, he joined the Mathematics and Computer Science department at Argonne National Laboratory (ANL), where he was an Assistant Computational Mathematician, and a Fellow in the Computation Institute at University of Chicago, becoming a Senior Research Associate in 2009. In 2015, he joined the Computational and Applied Mathematics department at Rice University. His research focuses on scientific computation, including scalable algorithms and parallel computing, numerical analysis, software development, high dimensional function approximation, and computational geophysics and biology. He is an author of the widely used PETSc library for scientific computing from ANL, and is a principal designer of the PyLith library for the solution of dynamic and quasi-static tectonic deformation problems. He developed the PETSc scalable unstructured mesh support based upon ideas from combinatorial topology. He was a J. T. Oden Faculty Research Fellow at the Institute for Computation Engineering and Sciences, UT Austin, in 2008, won the R&D 100 Award in 2009, and the SIAM/ACM Prize in Computational Science and Engineering in 2015 as part of the PETSc team.

# Numerical Continuation for Random and Stochastic Differential Equations

*C. Kühn* [1]

[1]School of Computation Information and Technology, Department of Mathematics, Technical University of Munich, Garching bei München, Germany

Topic: Stochastic Models, Uncertainty Quantification & Inverse Methods

**IS**

Uncertainty frequently arises in complex systems to resolve microscopic or external processes. Yet, the analysis of the resulting models carries a significant additional challenge of dimensionality. In this talk, I shall explain how to lift numerical continuation methods that are one of the most common and dimension-friendly tools in the applied sciences to understand nonlinear dynamics to random differential equations as well as to stochastic differential equations. The key idea is to obtain deterministic governing equations for key observables and then exploit these directly inside predictor-correct schemes. This is joint work with several colleagues, see e.g. [1-5].

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**About:**

The research interests of Christian Kühn lie at the interface of differential equations, dynamical systems and mathematical modelling. A key goal is to analyze multiscale problems and the effect of noise/uncertainty in various classes of ordinary, partial, and stochastic differential equations as well as in adaptive networks. The phenomena of central interest are: patterns, bifurcations and scaling laws. On a technical level, Kühn's work aims to build bridges between different areas of the study of dynamical systems. After studying mathematics at Jacobs University Bremen (BSc 2005) and at the University of Cambridge (M.A.St. 2006), Kühn received his PhD in Applied Mathematics from Cornell University in 2010. Subsequently he worked at the Max Planck Institute for the Physics of Complex Systems in Dresden as a postdoctoral researcher in the field of network dynamics. From 2011 to 2016 he was postdoctoral fellow at Vienna University of Technology in the Institute for Analysis and Scientific Computing and a Leibniz fellow at MFO in 2013. He is Lichtenberg Professor at TUM (starting 2016 as Assistant Professor and from 2022 Full Professor).

## Instability and equilibration of fluid-mineral systems under stress investigated through molecular dynamics

*M.L. Mazzucchelli*[1], *E. Moulas*[2], *S.M. Schmalholz*[1], *B.J.P. Kaus*[2], *T. Speck*[3]

[1]Institute of Earth Sciences, University of Lausanne, Lausanne, Switzerland; [2]Institute of Geosciences & Mainz Institute of Multiscale Modeling (M3ODEL), Johannes-Gutenberg University, Mainz, Germany; [3]Institute for Theoretical Physics IV, University of Stuttgart, Stuttgart, Germany

Topic: Multiscale Methods, Interdisciplinary Applications **CT**

Stress gradients and non-hydrostatic stresses are to be expected in rocks in the lithosphere, even in the presence of fluids. This complexity challenges the reliability of existing hydrostatic thermodynamic models, and, currently, in the geological literature there is still no accepted theory for evaluating the thermodynamic effects of non-hydrostatic stress on reactions [e.g. 1]. Large-scale Molecular Dynamics (MD) simulations (i.e., >2e6 atoms) allow us to investigate reactions in deforming systems by directly bridging the scale between atomic-level processes and continuum deformation. With MD, the a-priori assumption of a specific thermodynamic potential is not required, which makes it a robust approach to test existing thermodynamic theories [2]. Our findings indicate that a solid under non-hydrostatic stress can be equilibrated with its pure fluid. However, in the presence of substantial non-hydrostatic stresses, the stressed system becomes unstable, leading ultimately to the precipitation of a quasi-hydrostatically stressed crystalline film on the surfaces of the initial highly stressed crystal. During crystallization, the total stress balance is preserved until the newly formed solid-film-fluid system reaches again a stable equilibrium. At the final equilibrium conditions only the low-stressed solid film is exposed to the fluid, restoring the fluid pressure to a value close to that expected under homogeneous hydrostatic conditions. While our results agree qualitatively and quantitatively with previous theories of thermodynamics in deformed systems [3,4] and with experiments, they cannot be predicted by the theories currently proposed to interpret reactions in deformed geological systems [e.g., 1].

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# Machine Learning-Based Collective Variables and a Graph Neural Network Approach for Targeted Dynamics and Free Energy Manipulation in Molecular and Material Systems

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[1]Department of Chemical Engineering, Technion Israel Institute of Technology, Haifa, Israel

Topic: Interdisciplinary Applications, HPC & Machine Learning **IS**

Enhanced sampling techniques are essential for addressing rare-event limitations in molecular dynamics simulations of complex systems. Methods such as Umbrella Sampling, Metadynamics, and Adaptive Biasing apply biasing potentials along carefully chosen collective variables (CVs) to accelerate transitions across free energy barriers. However, identifying effective CVs remains a significant challenge. Recent advances relying on the use of machine learning have introduced powerful strategies for automating and improving CV discovery. In this talk, we present a methodology that leverages machine-learned CVs requiring minimal prior information for purposefully reshaping the free energy landscapes of considered systems, enabling control over their thermodynamic and kinetic behaviours. We further explore the use of a graph neural network-based simulator for enhanced sampling and efficient system-to-property learning, highlighting its potential to engineer the dynamics and functionality of complex molecular systems.

**About:**

Dan Mendels is an Assistant Professor at the Wolfson Department of Chemical Engineering at the Technion - Israel Institute of Technology. Before joining the Technion, he was a postdoctoral scholar at the Pritzker School of Molecular Engineering at the University of Chicago, where he focused on the design and engineering of smart materials. Prior to that, he held a joint postdoctoral appointment at USI and ETH Zurich in Switzerland, concentrating on the development of enhanced sampling methodologies. Dan holds a Ph.D. in Electrical Engineering from the Technion and an M.Sc. and B.Sc. in Physics with Honors, from the Hebrew University of Jerusalem. His research group develops and applies computational and machine learning-based tools for enhanced sampling in atomistic simulations, with applications in the design of systems such as smart materials, proteins and macromolecules.

## Modeling the origin of Eukarya

*E.M. Muro*[1], *F.J. Ballesteros*[2], *B. Luque*[3], *J. Bascompte*[4]

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Topic: Multiscale Methods, Interdisciplinary Applications **CT**

The origin of Eukarya is one of the most important events in the history of life on Earth. The endosymbiotic theory is widely accepted, but there is a gap of evolutionary intermediates. This is often described as "the black hole at the heart of biology". Here we model how life's genetic architecture was transformed to enable such a dramatic increase in complexity. To achieve this, we bring together computational biology, evolutionary biology, and physics. Our analysis revealed that the lengths of proteins and their corresponding genes follow lognormal distributions arising from multiplicative stochastic processes across the whole tree of life. We identified a scale-invariant relationship between mean gene length and variance. Finally, we found a second order phase transition in the emergence of the eukaryotic cell. The transition was driven by a tension between the evolutionary pressure to increase gene length and the limitations of producing longer proteins. The origin of the eukaryotic cell occurred at a critical and observable point that paved the way for other major evolutionary transitions that have shaped life on Earth as we know it today [1,2,3].

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## Localized model reduction for multiscale problems with application in PDE constrained optimization

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Topic: Multiscale Methods **IS**

Model order reduction for parameterized partial differential equations is a very active research area that has seen tremendous development in recent years from both theoretical and application perspectives. A particular promising approach is the reduced basis method that relies on the approximation of the solution manifold of a parameterized system by tailored low dimensional approximation spaces that are spanned from suitably selected particular solutions, called snapshots. With speedups that can reach several orders of magnitude, reduced basis methods enable high fidelity real-time simulations for certain problem classes and dramatically reduce the computational costs in many-query applications. While the "online efficiency" of these model reduction methods is very convincing for problems with a rapid decay of the Kolmogorov n-width, there are still major drawbacks and limitations. Most importantly, the construction of the reduced system in a so called "offline phase" is extremely CPU-time and memory consuming for large scale or multiscale systems. For practical applications, it is thus necessary to derive model reduction techniques that do not rely on a classical offline/online splitting but allow for more flexibility in the usage of computational resources.

In this talk we focus on both, localized training and on-the-fly enrichment strategies [1] for localized model order reduction of multiscale problems in the context of PDE constrained optimization [2,3]. The approaches are based on the reduced basis - trust region framework, recently developed in [4,5]. Concepts of rigorous certification and convergence will be presented, as well as numerical experiments that demonstrate the efficiency of the proposed approaches.

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**About:**
Mario Ohlberger is a full professor of applied mathematics and managing director of Applied Mathematics: Institute of Analysis and Numerics at the University of Münster. He is a member of the Center for Data Science and Complexity as well as the Center for Multiscale Theory and Computation. Since 2019 he is one of the spokespersons of the Cluster of Excellence Mathematics Münster: Dynamics - Geometry - Structure. His research area is numerical analysis for partial differential equations with a particular focus on error control and adaptivity, model order reduction, numerical multi-scale methods, scientific machine learning and scientific computing.

## Spontaneous strain and reactive fluid flow localization in space and time: interplay between continuum mechanics model formulations, numerical algorithms and HPC

*Y. Podladchikov*[1]

[1]Geocomputing Centre, University of Lausanne, Lausanne, Switzerland

Topic: HPC & Machine Learning

CT

Predictive modeling of timing and spatial location of strain and fluid flow localization events requires high numerical resolution both in space and in time to check for potential locations of the events. HPC parallel algorithms and use of GPU accelerators allows over two orders of magnitude speedup on a single card and linear scaling up thousands of GPU cards. Model formulations must be in the divergent form to allow for spontaneous development of discontinuities. Numerical algorithms must be conservative and consistent. True or pseudo- transient iterative techniques are required to treat the path-dependent processes such as pressure sensitive plastic shear banding. Utilization of the local and explicit conservative finite difference discretization is the simplest, and, possible, the only way to achieve all the above-mentioned goals.

## Using the Julia language to tackle portability and differentiable modelling at scale

*L. Räss*[1]

[1]Geocomputing Centre, University of Lausanne, Lausanne, Switzerland

Topic: HPC & Machine Learning, Uncertainty Quantification & Inverse Methods **IS**

The Julia language has gained significant traction in high-performance computing (HPC) due to its ability to overcome the traditional two-language barrier, offering the ease of high-level programming without compromising performance. With the rise of GPUs and other accelerators, the HPC landscape has shifted significantly, yet achieving both performance and portability across diverse backends remains a major challenge. Julia's powerful GPU ecosystem allows for the development of high-performance code targeting multiple architectures, while maintaining code conciseness and modularity.

Beyond GPU computing, one of Julia's standout features is its native support for automatic differentiation (AD). Thanks to tools like Enzyme.jl, an AD framework integrated directly with the LLVM compiler, it is now possible to combine differentiation with compiler-level optimisations. This enables highly efficient reverse-mode AD, approaching theoretical peak performance.

In this talk, I will explore the benefits and challenges of using Julia in an HPC context. I will highlight how Julia enables seamless transitions from prototyping to production, supports execution across various hardware backends, and allows for full-program differentiation, including multi-GPU applications, using a single, unified codebase.

**About:**

Ludovic Räss is a computational geoscientist at the University of Lausanne and a lecturer at ETH Zurich. His research sits at the intersection of high-performance computing, geophysics, and applied mathematics, with a focus on GPU-accelerated scientific computing. He studies spontaneous flow localisation in deforming porous media and ice dynamics, and develops portable, scalable HPC software for diverse computing architectures. He leads the GPU4GEO initiative, advancing GPU-based multi-physics solvers. His recent work explores differentiable modelling and large-scale optimisation, developing differentiable multi-physics solvers in Julia, with active contributions to the JuliaGPU and JuliaParallel ecosystems.

# Machine-learning accelerated catalyst discovery and characterisation

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Topic: HPC & Machine Learning, Multiscale Methods **IS**

The discovery and characterization of efficient catalysts remains a challenge due to the complex structure of nanoparticle-based heterogeneous catalysts. State-of-the-art screening approaches often rely on single adsorption energies as descriptors of catalytic activity, which neglect the variation across different surface facets and binding sites. To facilitate catalyst discovery, we introduce the adsorption energy distribution (AED), a descriptor that captures the full spectrum of adsorption behavior across a catalyst material, thereby extending the Sabatier principle to realistic nanostructured materials [1]. To accelerate AED generation, we used machine-learned interatomic potentials (MLIPs) from the Open Catalyst Project [2]. We built a scalable workflow starting from bulk metals or alloys, generating stable surfaces, identifying all binding sites, and computing AEDs. Using hierarchical clustering, we classified catalysts for CO2 to methanol conversion based on AEDs and uncover promising candidates such as ZnRh or ZnPt3 [1]. Regarding characterization, we have developed active learning workflows to train MACE MLIPs to generate infrared (IR) spectra of catalytically relevant molecules. Our MLIPs provide accurate IR spectra at a fraction of the computational cost of the conventional density-functional theory-based IR approach and can now be used to generate data for inference models of in-situ IR experiments.

References:

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[2] https://opencatalystproject.org/

**About:**

Patrick Rinke received his PhD from the University of York in England in 2003. He was then a post-doctoral scholar at the Fritz Haber Institute (FHI) of the Max Planck Society in Berlin and in the Materials Department at the University of California Santa Barbara (UCSB) before becoming a group leader at the FHI in 2009. In 2014, he was appointed Professor for Computational Electronic Structure Theory in the Department of Applied Physics at Aalto University in Helsinki, Finland. Since 2024, he leads the AI-Based Materials Science Chair at Technical University Munich. He develops advanced electronic structure, data science and machine learning methods and applies them to pertinent problems in materials science. In 2023 he received the Aalto Open Science award for creating the Aalto Materials Digitalization platform AMAD.

## High order Asymptotic-Preserving penalized numerical schemes for the Euler-Poisson system in the quasineutral limit

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Topic: Multiscale Methods **CT**

In this talk, we present the development of a new class of numerical methods able to both handle quasineutrality and charge separation in plasmas. At large temporal and spatial scales, plasmas tend to be quasineutral, which means the local net charge density is nearly zero. However, when the scale at which one observes the plasma dynamics is smaller than the characteristic distance over which the electric field and charges are typically screened, then quasineutrality breaks down. In such regimes, standard numerical methods face severe stability constraints, rendering them practically unusable. To address this issue, in this work, we introduce and analyze a new class of finite volume penalized-IMEX Runge-Kutta methods for the Euler-Poisson (EP) system, specifically designed to handle the quasineutral limit. The design is based on the introduction of a penalization term which enables us to get a density that inturn stabilizes the Poisson equation. We show that, these proposed schemes are uniformly stable with respect to the Debye length and degenerate into high order methods as the quasineutral limit is approached. Several numerical tests confirm that this new class of methods exhibits the desired properties.

## Application of machine learning techniques to differential equations

*M. Lukáčová-Medvidová*[1], *S.T. Nguyen*[1], *S. Schneider*[1], *P. Spichtinger*[2]

[1]Institute of Mathematics, Johannes Gutenberg University, Mainz, Germany; [2]Institute for Atmospheric Physics, Johannes Gutenberg University, Mainz, Germany

Topic: HPC & Machine Learning

CT

In this talk we present our recent work on the application of machine learning techniques to differential equations. In the first part, we present a machine learning based approach for a reduced model of warm clouds used in atmospheric applications. In the second part, we use neural networks as trial functions in the context of partial differential equations. For hyperbolic conservation laws we present rigorous convergence analysis for a suitable network architecture. The present research has been done in cooperation with M. Lukáčová-Medvidová, P. Spichtinger and S.T. Nguyen and supported by M3ODEL.

## A hybrid multiscale method for the simulation of ring polymers

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[2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Topic: Multiscale Methods, Interdisciplinary Applications **CT**

In our work [1], we develop a hybrid multiscale model to describe the flow behavior of dense melts of semiflexible and flexible ring polymers in the presence of walls. Our considerations are motivated by the molecular dynamics (MD) simulations presented in [2]: Polymer melts as described above do not separate in equilibrium. The introduction of walls does not change this. If, however, the mixture is additionally subjected to flow, the polymers start to segregate.

Our model consists of a set of continuum equations that include microscale information derived from MD simulations. More precisely, we consider a Cahn-Hilliard-Navier-Stokes system with a stress tensor obtained from MD simulations via an averaging procedure. A similar approach for single-component flows has been pursued in [3] and [4]. We present a suitable finite-element discretization of our equations yielding a mass conserving and energy stable numerical scheme and show numerical results.

This work has been supported by the DFG (Deutsche Forschungsgemeinschaft) via the SFB/TRR 146 "Multiscale Simulation Methods for Soft Matter Systems".

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## The Role of Simulation Scale in Modeling Water Transport to the Upper Atmosphere

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[1]Institute for Atmospheric Physics, Johannes Gutenberg University, Mainz, Germany

Topic: Interdisciplinary Applications CT

Warm conveyor belts (WBCs) are large-scale ascending air streams found in extratropical cyclones. They have been identified as a major source of water vapour (a potent greenhouse gas) and hydrometeors in the upper troposphere/lower stratosphere (UTLS), which can form cirrus clouds that also influence the climate. Therefore, WCBs play an important role in the Earth's radiative budget. Additionally, they transport large amounts of heat across latitudes and can influence the circulation of the upper troposphere after they dissipate, which highlights their importance for the weather and climate of the Earth. Recent studies using high-resolution, convection-permitting simulations have shown that air often ascends rapidly in WCBs through convection. These air parcels transport significantly more hydrometeors into the UTLS than slower-ascending air parcels. Furthermore, cloud and precipitation development in convective air parcels is dominated by different processes to those in air that ascends more slowly. However, the global numerical weather prediction and climate models that are commonly used to assess the climatological and future impacts of WCBs operate at grid resolutions of 15-50 km, which are not convection-permitting. Instead, these models rely on convection parameterisation schemes. The Tiedtke-Bechtold convection parameterisation scheme, which is widely used, is designed to simulate heat, moisture and momentum transport in convective systems, but it only includes basic representations of cloud microphysics. This raises the question of whether low-resolution simulations accurately represent the transport of hydrometeors into the UTLS by WCBs compared to highresolution, convection-permitting simulations. To address this issue, we analysed two simulations of the same WCB — one convection-permitting and one using convection parameterisation — with a specific focus on vapour and hydrometeor transport. Our results show that the WCB in the high-resolution simulation transports substantially larger amounts of hydrometeors into the UTLS and alters their vertical distribution. In the higher-resolution simulation, the UTLS is drier than the lower-resolution simulation in certain regions, and more moist in others. Depending on the grid scale, microphysical processes also shift from liquid-dominated to frozen-dominated when the resolution is higher.

## Element learning: accelerating finite element-type methods via machine learning, and application to radiative transfer

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[2] Syracuse University, Syracuse, USA

Topic: HPC & Machine Learning; Interdisciplinary Applications **IS**

In numerical simulations of complex multiscale systems, a significant challenge is computational expense. To speed up computations, artificial neural networks and machine learning tools have surfaced as game changing technologies. However, many machine learning approaches tend to lose some of the advantageous features of traditional numerical PDE methods, such as interpretability. In this talk, we introduce a systematic approach (which we call element learning) with the goal of accelerating finite element-type methods via machine learning, while also retaining the desirable features of finite element methods.

For an example application, numerical tests are presented for radiative transfer. Our long-term goal is to break the 1D barrier and enable 3D radiative transfer calculations, for weather and climate applications, accelerated by both element learning and hp-adaptive mesh refinement. Element learning can accelerate computations by a factor of 5 to 20, for fixed degrees of freedom or a fixed accuracy level of $10^{-3}$ in the relative $L^2$ error. [1,2]

References:
[1] Du S., Stechmann S. arxiv.2308.02467 (2023)
[2] Du S., Stechmann S. J. Comp. Math. (2025) in press

**About:**

Sam Stechmann is Professor of Mathematics at the University of Wisconsin–Madison, and holds affiliate roles in the Department of Atmospheric & Oceanic Sciences as well as the Center for Climatic Research. He earned his Ph.D. in Mathematics from NYU's Courant Institute in 2008, after which he held a postdoc position at Los Alamos National Laboratory, where he deepened his expertise in applied mathematics for environmental systems. His research bridges applied and computational mathematics with atmospheric science, focusing on scientific machine learning, stochastic processes, multiscale modeling, numerical methods for PDEs, and radiative transfer to tackle complex climate processes like radiation, convection, and tropical dynamics.

## Error estimates and variance reduction for nonequilibrium stochastic dynamics

*G. Stoltz*[1,2]

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Topic: Stochastic Models **IS**

Equilibrium properties in statistical physics are obtained by computing averages with respect to Boltzmann–Gibbs measures, sampled in practice using ergodic dynamics such as the Langevin dynamics. Some quantities however cannot be computed by simply sampling the Boltzmann–Gibbs measure, in particular transport coefficients, which relate the current of some physical quantity of interest with the forcing needed to induce it. For instance, a temperature difference induces an energy current, the proportionality factor between these two quantities being the thermal conductivity. From an abstract point of view, transport coefficients can also be considered as some form of sensitivity analysis with respect to an added forcing to the baseline dynamics. There are various numerical techniques to estimate transport coefficients, which all suffer from large errors, in particular large statistical errors. I will review the most popular methods, namely the Green–Kubo approach where the transport coefficient is rewrittten as some time-integrated correlation function, and the approach based on longtime averages of the stochastic dynamics perturbed by an external driving (so-called nonequilibrium molecular dynamics). I will make precise in each case the various sources of errors, in particular the bias related to the time discretization of the underlying continuous dynamics, and the variance of the associated Monte Carlo estimators. I will also briefly present various recent alternative techniques to estimate transport coefficients.

**About:** Gabriel Stoltz is a researcher in applied mathematics at CERMICS, the applied mathematics center of Ecole nationale des ponts et chaussées, which is part of Institut Polytechnique de Paris. He is also currently the director of CERMICS. He obtained his PhD in 2007 and defended his habilitation thesis in 2012. His work focuses on the mathematical and numerical analysis of models from molecular simulation, with a current emphasis on computational statistical physics. This involves, from a mathematical viewpoint, techniques ranging from probability theory and the study of stochastic processes, to functional analysis and the theory of partial differential equations; as well as numerical analysis, scientific computing and machine learning.

## The microscopic origin of thermodynamic irreversibility

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Topic: Multiscale Methods **CT**

Macroscopic thermodynamics has a clear arrow of time, characterized by the monotonous increase of entropy during the approach to equilibrium. The microscopic laws of physics, on the other hand, are invariant under time reversal – whatever can happen in one direction of time is also possible in the other. Explaining this tension is a classical example for a multiscale modeling problem – how can a macroscopic system have properties seemingly in contradiction to those of its microscopic constituents? In this talk, I will explain how this challenge can be analyzed and (to some extend) resolved using multiscale modeling techniques, specifically the projection operator formalism [1].

References:

[1] te Vrugt M. Understanding probability and irreversibility in the Mori-Zwanzig projection operator formalism, European Journal for Philosophy of Science 12, 41 (2022)

## Control of nonlinear bulk deformation and large shear strain on first-order phase transformation kinetics

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Topic: Multiscale Methods **CT**

Phase transformations play a key role in numerous coupled natural processes, and they are important for many industrial applications. However, the kinetics of phase transformations in coupled chemo-mechanical systems undergoing large mechanical deformations still needs to be better quantified. Here, we study the phase transformation kinetics of a two-phase binary mixture using the diffuse interface approach. We couple a Cahn–Hilliard type model with a mechanical model for a compressible viscous flow. The bulk compressibility is a nonlinear function of the pressure, and the shear viscosity is a nonlinear function of the concentration. The mechanical coupling is achieved by employing a pressure-dependent mechanical mixing term in the equation for the Gibbs energy. We derive a dimensionless system of equations which we solve numerically with a pseudo-transient method using conservative finite differences for discretization. We perform numerical simulations in 1D and 2D model setups considering far-field simple shear and pure shear. For a chemo-mechanically coupled system, we show that the velocity of the phase boundary is a linear function of the degree of metastability and, hence, confirm the hypothesis of "normal growth." A stronger mechanical coupling and a larger volumetric effect of the chemical reaction result in lower phase boundary velocities. The 2D results show a significant impact of the mechanical coupling and the far-field deformation on the orientation and kinetics of the phase transformations. Under far-field simple shear and pure shear in 2D, the phase transformations generate string-like patterns. The orientation of these patterns is controlled by the applied far-field deformation and orientations differ by 45 degrees between simple shear and pure shear.

## Biomolecular condensates with a Twist: From Assembly to Arrest

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Topic: Multiscale Methods **CT**

Biomolecular condensates are phenomena that emerges through liquid-liquid phase separation of disordered proteins. In this work, we study one such protein known as Fused in Sarcoma (FUS), a multi-domain protein with regions rich in arginine and glycine residues, referred to as RG-rich domains, which are involved in a wide range of essential cellular processes. Unique sequence patterns such as RGGRGRGG...RGRGGGRGG.. allow FUS to interact with itself and with nucleic acids. The role of these repeats in phase separation can be significantly diminished by point mutations e.g., RtoK, RtoA, which disrupt the naturally occurring pattern. Although lysine carries a positive charge similar to arginine, it lacks the guanidine group, limiting its interaction network. The alanine substitution completely breaks the interaction network and impair the FUS's ability to form droplets. Beyond phase separation, we also investigate the time-dependent viscoelastic properties of FUS condensates as altered by mutations. In many cases, condensates that exhibit liquid-like (so called "Newtonian fluid") behavior transition into a non-Newtonian regime known as a Maxwell fluid, which exhibits elastic characteristics. From application point of view, Non-Newtonian condensates may act as a protein reservoirs that accelerate biochemical reactions. On the other hand, elastic or gel-like protein-RNA condensate could provide structural support to shape chromatin organization in the nucleus. Multi-resolution simulation models, one bead per residue (CALVADOS3), Martini3 and all-atom simulations are employed in order to capture the pronounced difference induced by the point mutations. Our current results appear to be in qualitative agreement with the experimental findings.

References:
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[3] Cao F., von Bülow S., Tesei G., Lindorff-Larsen K. Protein Science 33(11):e5172 (2024)
[4] Jawerth L., Hyman A.A., Jülicher F. Science 1317-1323 (2020)

## Kinetic modelling of non-equilibrium gas-particle partitioning in secondary organic aerosols: towards mass closure in atmospheric nanoparticle growth

*Z. Zhang*[1], *H.G. Kang*[1], *A. Mishra*[1], *M.W. Radecka*[1], *U. Pöschl*[1], *T. Berkemeier*[1]

[1]Multiphase Chemistry Department, Max Planck Institute for Chemistry, Mainz, Germany

Topic: Interdisciplinary Applications CT

Equilibration timescales of partitioning of semi-volatile compounds can be prolonged in highly viscous particles with diffusion limitations [1,2], and growth rates of ambient secondary organic aerosols (SOA) show little dependence on condensable vapors in the gas phase [3]. Low-volatility oxygenated organic molecules, critical to the survival of newly formed particles to cloud condensation nuclei, can lead to high viscosity and low diffusivity. SOA can be highly viscous, causing non-equilibrium partitioning and slowing nanoparticle growth. We apply a kinetic process model of aerosol chemistry and mass transport to estimate the diffusion limitations affecting the initial steps of condensational growth of SOA right after nucleation in the ambient atmosphere. The model explicitly accounts for the Kelvin effect, gas-particle partitioning, and bulk diffusivity. We compare the model with data from laboratory and field studies of nanoparticle growth [4]. The modeled partitioning of semi- and low-volatile organic compounds (SVOC/LVOC) is strongly affected by diffusion limitations, while the partitioning of extremely- and ultra-low volatility organic compounds (ELVOC/ULVOC) is less affected. Thus, considering the particle phase state and bulk diffusion coefficients may lead to a better mass closure in models of atmospheric nanoparticle growth. The results provide new insights into the condensational growth of newly formed molecular clusters, which is crucial for the climate relevance of new particle formation.

References:
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# Poster Presentations

## Small scale caldera collapse - A numerical study on central vent caldera-forming eruptions

*P.S. Aellig*[1,2], *A. de Montserrat Navarro*[3], *B.J.P. Kaus*[1,2]

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Topic: Interdisciplinary Applications

Large-scale magmatic systems are commonly associated with catastrophic caldera-forming eruptions. These events are generally linked to faults or eruption channels located at the periphery of the magma chamber, resulting in a caldera that reflects almost the full spatial extent of the reservoir. However, the dynamics of small to intermediate -scale magmatic systems that have also hosted caldera-forming eruptions, such as Krakatau (Indonesia) or Crater Lake (USA), are comparatively less explored. In these instances, the eruption is generally assumed to have begun from a single central vent of a volcanic edifice rather than through a ring fault system. In this study, we utilise a multi-physics numerical modelling approach to investigate the mechanics of central vent eruptions on the collapse stage. The interactions between magma dynamics, far-field tectonic stresses and non-linear visco-elasto-plastic rheologies are examined using the thermo-mechanical geodynamic code JustRelax.jl, in order to investigate the potential for roof failure above a shallow magma chamber. The models incorporate a thermally active magma chamber with variable geometries and a volcanic edifice. By simulating recharge of magma and volume depletion through eruptions, we thereby provide insights into the processes governing central vent-driven caldera formation. Here we present a systematic parameter study on the driving forces behind this type of caldera collapse.

# Integrating Behavioral Survey Data into Epidemic Models: A Methodological Framework

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Topic: Interdisciplinary Applications

Understanding the impact of human behavior on epidemic dynamics is an increasingly important direction in infectious disease modeling. While classical compartmental models such as SIR rely on fixed transmission parameters, real-world epidemics are shaped by dynamic behavioral factors—such as perceived risk, mask-wearing, or changes in mobility—often captured through survey-based data. This study aims to develop a mathematical modeling framework that integrates such behavioral survey data into an extended compartmental-type model, in order to capture feedback mechanisms between disease spread and adaptive human responses. Previous research has emphasized the importance of explicitly modeling the interplay between behavior and disease transmission. The work of Manfredi and d'Onofrio [1] provides a foundational basis for integrating behavioral dynamics into epidemiological models. Drawing from Bayesian approaches such as those proposed by Campbell et al. [2], behavioral indicators can be incorporated into time-varying transmission parameters. Reviews by Funk et al. [3] further outline how adaptive behavior influences epidemic outcomes, while the empirical framework of Tizzoni et al. [4] demonstrates how survey and epidemiological data can be jointly analyzed to reveal behavioral patterns during outbreaks. By connecting behavioral data with dynamic models of disease spread, this project contributes to a more realistic understanding of epidemic trajectories. The ultimate objective is to improve predictive accuracy and support public health decision-making through an integrated, behaviorally informed modeling approach.

References:

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[2] Campbell A.P., Koelle K., Holmdahl I. Bayesian modeling of dynamic behavioral change during an epidemic. PLOS Computational Biology, 17(6), e1009218. (2021) doi:10.1371/journal.pcbi.1009218

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## Overshooting convection over southern Scandinavia: a modeling perspective

*I. Bartolome Garcia*[1,2], *A. Miltenberger*[1], *P. Konjari*[2], *C. Rolf*[2], *M. Krämer*[1,2]

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Topic: Multiscale Methods, HPC & Machine Learning

Convective overshoots of cloud tops can transport water vapor into the upper troposphere-lowermost stratosphere (UTLS), where even small changes in the amount of water vapor can have a large impact on the radiative budget. Therefore, understanding the dynamics of the overshoots is crucial to properly represent them. A recent study by [1] analyses a convective overshoot observed on the 12.06.2024 over southern Scandinavia during the airborne TPex campaign using in-situ measurements, satellite observations and simulations. In our study, we perform a high-resolution simulation (400 m in the horizontal, 150 m in the vertical) of the same case with the ICOsahedral Nonhydrostatic (ICON) modeling framework. We focus on understanding the dynamics of the overshoot and the processes affecting the ice microphysics. For this analysis, we use the ice modes from [2] that differentiate between five formation mechanisms.

References:
[1] Konjari et al. (2025)
[2] Lüttmer et al. (2024)

## Ice clouds as nonlinear oscillators

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[1]Institute for Atmospheric Physics, Johannes Gutenberg University, Mainz, Germany

Topic: Multiscale Methods, Interdisciplinary Applications

Clouds are important features of the atmosphere, determining the energy budget by interacting with incoming solar radiation and outgoing thermal radiation, respectively. For pure ice clouds, the net effect of radiative effect is still unknown. In this study we develop a simple but physically consistent ice cloud model, and analyze it using methods from the theory of dynamical systems. We find that the model constitutes a nonlinear oscillator with two Hopf bifurcations in the relevant parameter regime. In addition to the characterization of the equilibrium states and the occurring limit cycle, we find scaling behaviors of the bifurcations and the limit cycle, reducing the parameter space crucially. Finally, the model shows very good agreement with real measurements, indicating that the main physics is captured and such simple models are helpful tools for investigating ice clouds.

## Kinetic Modeling and Optimization of Soot Gasification Processes

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Topic: Multiscale Methods, Uncertainty Quantification & Inverse Methods

Soot gasification plays a critical role in various environmental and industrial processes, such as combustion technologies, emission control systems, and atmospheric aerosol chemistry. Despite its importance, the detailed mechanisms governing soot reactivity with oxidizing and gasifying agents remain poorly understood due to the complexity of multiphase interactions and the diversity of reaction environments. In this work, we employ the KM-GAP kinetic multilayer model [1] to simulate the gasification of soot in the presence of $NO_2$, $O_2$, $CO_2$, and water vapor. KM-GAP treats explicitly all steps of mass transport and chemical reaction of semi-volatile species partitioning between the gas phase, particle surface, and particle bulk. By fitting the model to experimental observations, we explore different reaction mechanisms and identify key parameters that influence the reactivity of soot surfaces, including activation energies and reaction rate coefficients. To improve parameter constraint, we employ the numerical compass (NC) [2] - a framework based on ensemble modeling and uncertainty quantification. Using NC, we identify optimal experimental conditions that maximize the potential to reduce parametric uncertainty and distinguish between competing reaction pathways.

References:
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[2] Krüger M. et al. (2024)

## Direct Molecular Polarizability Prediction with Local Frame GNNs on QM7-X

*J.P. Filling*[1], *M. Wand*[1]

[1]Institute for Computer Science, Johannes Gutenberg University, Mainz, Germany

Topic: HPC & Machine Learning

We propose a novel equivariant graph neural network (GNN) architecture for the direct prediction of molecular polarizability tensors using local coordinate frames. While most existing approaches regress scalar properties and rely on derivatives to obtain tensors, our method directly models rank-2 tensor outputs in a frame-consistent and physically meaningful way. By combining scalar, vector, and tensor channels within a local message-passing framework, our network captures rich geometric information while maintaining SE(3)-equivariance. We evaluate our model on the QM7-X dataset, focusing on the subset of optimized molecular geometries. This is a work in progress and represents a step toward more structured, geometry-aware neural models for covariant response properties.

## Realizing Quantitative Quasi-Particle Simulations of Skyrmion Dynamics in Arbitrary Potentials

*S.M. Fröhlich*[1], *M.A. Brems*[1], *T. Sparmann*[1], *L.-C. Dany*[1], *J. Rothörl*[1], *F. Kammerbauer*[1], *E.M. Jefremovas*[2], *O. Farago*[3], *M. Kläui*[1], *P. Virnau*[1]

[1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany; [2]Department of Physics & Materials Science, University of Luxembourg, Luxembourg; [3]Biomedical Engineering Department, Ben Gurion University of the Negev, Be'er Sheva, Israel

Topic: Multiscale Methods

Magnetic skyrmions are two-dimensional whirls of magnetization which can be topologically stabilized in thin films and visualized with magneto-optical Kerr microscopy. Skyrmions can exhibit thermal diffusion in a spatially inhomogeneous effective energy landscape that stems from pinning effects caused by random material defects [1]. They are also easy to manipulate which makes them promising candidates for novel devices in the context of unconventional computing [1, 2] and for the study of phase transitions in two dimensions [3]. In the so-called Thiele framework, skyrmions are described as two-dimensional quasiparticles which evolve according to an overdamped Langevin equation similar to chiral colloidal systems. In previous work, we have obtained effective interactions between skyrmions and boundaries using Iterative Boltzmann Inversion on experimentally determined radial distribution functions [4]. Here, we exploit experimentally observed diffusion of magnetic skyrmions in pinning potentials to realize fully quantitative Thiele model simulations on experimentally relevant time and length scales [5]. By determining the underlying pinning landscape, we can calibrate experimental and simulation time scales and current-induced forces.

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## High-Resolution Geodynamic Modeling of Volcanic Flank Instabilities Using HPC

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Topic: HPC & Machine Learning

The eastern flank of Mount Etna is currently sliding seaward at several centimeters per year. To assess the potential for accelerated failure, we develop a 3D visco-elasto-plastic model using LaMEM, a parallel finite-difference code optimized for HPC. The model incorporates high-resolution topography, seismic tomography, and GPS data to simulate deformation processes in a 43,000 $km^3$ domain at 50-meter resolution. Simulations involve large grids (e.g., 1000×1000×256) and time-dependent nonlinear rheologies, requiring access to EuroHPC resources. Preliminary runs on LUMI-C confirm the scalability of LaMEM at target resolution. A systematic parameter study is planned to identify the key controls on flank motion. This work supports hazard assessment for Etna and contributes to the development of reproducible, high-resolution geodynamic workflows. It is part of the ChEESE-2P project addressing exascale computing challenges in the solid Earth sciences.

## How can viscosity affect organic aerosol volatility derived from evaporation and thermal desorption measurements?

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Topic: Interdisciplinary Applications

Air quality models use experimentally derived volatility basis sets to parameterize secondary organic aerosol (SOA) formation [1]. Evaporation in a chamber or thermal desorption experiment, such as with the filter inlet for gases and aerosols coupled to a chemical ionization mass spectrometer (FIGAERO-CIMS), are common methods for estimating the volatility of SOA [2,3]. The thermograms from the FIGAERO-CIMS are often compared against empirical calibrations to retrieve the volatility distribution [3]. However, observations suggest that particle phase state affects interpretations of SOA volatility. For instance, the isothermal evaporation of SOA has been found to be insensitive to particle size [4], which cannot be explained with equilibrium partitioning theory. In experiments where SOA from different alkanes grew on dioctyl sebacate (DOS) seed, the thermal desorption temperature of the DOS increased with higher SOA viscosity [5]. We use the kinetic multilayer model of multiphase chemistry (KM3C) to address the impact that particle viscosity has on the evaporation and thermal desorption of SOA. KM3C divides the bulk of a SOA particle into layers, and thus is able to resolve bulk diffusion gradients. The model explicitly accounts for chemical kinetics, mass transport between the bulk layers, and gas-particle partitioning [6]. We use a relationship between vapor pressure and self-diffusivity as well as a logarithmic mixing rule to calculate the diffusivity of each layer based on the composition. We find that volatility distributions from isothermal evaporation data may be skewed towards the low-volatile side due to formation of a "surface crust". For the FIGAERO-CIMS, SOA desorbs at higher temperatures if particle viscosity is accounted for. We find that the effects of particle phase state should be addressed when interpreting SOA volatility from such data.

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## Numerical weather forecasting with Julia

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Topic: HPC & Machine Learning

I will give an overview on my success to incorporate known and new numerical methods for numerical weather predictions in one code base. The programming is done in the Julia language. All numerical methods are based on a common grid structure which starts from two dimensional grids (plane, sphere) and extruded in the third dimension. Parallel computation is done with two-dimensional domain decomposition and MPI. The main time loop after initialization is programmed with KernelAbstractions.jl which allows to use different backends like classical CPU's and different type of accelerators like Nvidia, AMD and other ones.

I will report on two implementation. The first one, following the HOMME code, is a spectral continuous element in the horizontal and finite differences in the vertical. The second one is a discontinuous Galerkin method in all three space directions. The two methods are compared for the baroclinic wave instability test example for different grid resolutions and number of used processing units.

## Asymptotic and Machine Learning Parameterization of the Effect of Gravity Waves on Ice Clouds

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Topic: HPC & Machine Learning, Multiscale Methods

Cirrus clouds, which make up around 30% of global cloud cover, play a crucial role in the radiation budget and influence climate sensitivity by approximately 20%. Their radiative properties strongly depend on microphysical factors such as ice crystal concentration. In this work, an existing asymptotic model is further developed to calculate the saturation ratio and the ice crystal concentration in cirrus clouds under the influence of monochromatic gravity waves. To achieve this, the second order of the asymptotic equations is derived and solved. The resulting model enables a more precise simulation of the saturation ratio and the resulting ice crystal concentration in cirrus clouds. In ongoing research, we aim to reproduce these results using machine learning techniques to model the evolution of the large-scale ice fields by using as input the small-scale gravity wave fluctuations.

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## Speed limits in terms of two entropy productions in a discretetime Markov chain

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Topic: Stochastic Models

A discrete-time Markov chain can serve as an effective modeling framework in several scenarios. First, it is well-suited for systems that are naturally observed or recorded at discrete time intervals. Second, it offers a universal platform for some kinds of continuous-time processes. Third, when the primary quantities of interest are based on discrete time steps. Finally, in cases where the system's dynamics themselves are triggered or evolve in discrete steps. In this research we investigated the two types of entropy production, the time-backward entropy production and the timereversed entropy production, and we derived an entropic inequality which is the so-called speed limit for each entropy production. Since our research extends the speed limits from the continuous-time regime to the discrete-time regime, it significantly broadens the applicability of thermodynamic speed limits. We verified our results on physical examples including breast cancer cell dynamics.

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## Hamiltonian Monte Carlo applied in inverse petrological modeling

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Topic: Uncertainty Quantification & inverse Methods, Interdisciplinary Applications

Metamorphic rocks represent physical systems that record complex dynamic histories in which temperature and pressure evolve over time. The evolution of such rocks may be investigated with the use of distinct inverse modeling approaches. The output of such models is compared with natural observations such as geochronological or mineral compositional data. This comparison between modeled and natural data allows the estimation of key parameters like the effective cooling rate. These parameters help constrain the timescales of geological processes such as exhumation. However, the observed data often include random or systematic errors. Therefore, it is important to evaluate how these uncertainties are reflected in the estimated inverse parameters. In this work, we focused on the metamorphic sole of the Pindos ophiolite in northwestern Greece. Based on previously obtained geochronological and thermobarometric data, we derive effective cooling rates through a combination of inversion techniques. Specifically, we employed a non-linear, multicomponent diffusion model to reproduce observed compositional gradients in garnet by finding an optimal cooling rate relevant to the near-peak conditions. In addition, 40Ar/39Ar ages of muscovite from a metapelite and hornblende from an amphibole of the Pindos metamorphic sole were fit using a similar diffusion approach to obtain an effective cooling rate. To quantify the uncertainties of the inverted parameters we apply, for the first time in inverse petrological modeling, the Hamiltonian Monte Carlo (HMC) method. Our study shows that combining multiple inversion methods with petrological data and uncertainty quantification is advantageous for elucidating the complex evolution of metamorphic rocks.

## A coarse-grained model for SMC-mediated DNA loop extrusion

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Topic: Interdisciplinary Applications

Structural maintenance of chromosome (SMC) complexes are involved in genome organization and regulation via DNA loop extrusion. During extrusion SMC proteins reel DNA from one or both sides and a loop forms and increases. Our collaboration partners investigate this process by grafting l-DNA onto a plate and exposing it to SMC proteins. To model this process in simulations, we propose a coarse-grained model for DNA loop extrusion using a Kratky-Porod chain as a basis for DNA. We show that our model reproduces knotting probabilities from DNA experiments as a function of chain length and ionic solvent conditions, which can be considered a fine gauge for structural properties [1]. SMC proteins are modelled as handcuffs through which the DNA is pulled. The coarse-grained nature of our model enables us to perform simulations at experimental time and length scales by matching forces at which extrusion stalls. At low DNA tension, Smc5/6 and Wadjet extrude DNA from both sides of the loop. At higher tension, however, they transition to a behavior akin to one-sided extruders, yet still capable of extruding from one or the other side thereby switching the direction of extrusion [1]. By combining experiments and simulations, we explain this behavior as a complex interplay of extrusion, stalling and thermal fluctuations.

## Scalable hybrid multigrid for staggered grid discretizations in geodynamics

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Topic: HPC & Machine Learning

The staggered grid finite difference discretization demonstrates a good scalability on parallel machines with a coupled multigrid preconditioner based on Galerkin coarsening scheme. However, it relies on the assembled matrices with a significant memory imprint, which prohibits achieving peak performance. A geometric multigrid method poses a valuable alternative, since an increased number of iterations can be compensated by a greater performance of the matrix-vector products computed in a matrix-free manner. Here we present a hybrid multigrid framework that allows optimal combination between various types of coarsening techniques for staggered grid discretizations. Our implementation follows the approach suggested previously for the finite element discretizations [1]. Here, we extend it to the staggered grid finite difference, discuss the optimal solver parameter selection, and document performance gains that can be achieved by using the matrix-free operators. We typically start with a few levels of re-discretized matrix-free operators, followed by Galerkin geometric coarsening operating on assembled matrices. At the coarse grid level, we either utilize a parallel sparse direct solver or a black-box algebraic multigrid method. The number of processors participating in a coarse grid solve can be optimally selected via PETSc sub-communicator framework (Telescope) [2].

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## Numerical Simulations of Blood Flow in Realistic Human Arteries for the Assessment of Patient Specific Risk

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Topic: Interdisciplinary Applications

Cardiovascular diseases remain a leading cause of mortality, yet current risk assessment methods lack patient-specific precision. In our research we develop in collaboration with Universitätsmedizin Mainz validated numerical models using Computational Fluid Dynamics (CFD) and Fluid-Structure Interac-tion (FSI) to enable personalized cardiovascular risk assessment in human arteries, particularly focusing on carotid arteries and aortas. Patient-specific arterial geometries are reconstructed from high-quality CT Angiography (CTA) scans and processed using automated segmentation tools. Advanced FSI simulations incorporate realistic arterial compliance through strain-dependent material properties derived from in vitro experiments on silicon arterial phantoms [1]. Novel time-dependent resistance boundary conditions accurately model physiological pressure waves and the Windkessel effect, replacing conventional zero-stress assumptions [1]. The models evaluate established hemodynamic risk indicators including Wall Shear Stress (WSS) and Oscillatory Shear Index (OSI) [2]. Our investigation demonstrates that patient-specific simulated OSI successfully predicts sites of aortic dissection when comparing pre- and post-dissection states. Histological analysis conducted from Universitätsmedizin Mainz confirms tissue degradation in numerically predicted high-shear zones.

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## A kinetic model of multiphase chemistry integrating size distribution dynamics in secondary organic aerosol formation

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Topic: Interdisciplinary Applications

Secondary organic aerosols (SOA) are one of the largest natural and anthropogenic aerosol sources. However, there still remain discrepancies between the growth rates of nanoparticles measured in the laboratory, the ambient atmosphere, and those predicted in model calculations [1]. Furthermore, there is a lack of kinetic models that explicitly describe particle-phase diffusion and chemistry, as well as new particle formation (NPF) and size distribution dynamics. We use the kinetic multilayer model for multiphase chemistry (KM3C) and investigate the evolution of particle size distributions during oxidation of $\alpha$-pinene and limonene with the $NO_3$ radical in the presence of seed aerosol in a laboratory chamber, as well as the ozonolysis of oleic acid. KM3C explicitly treats gas-phase chemistry, gas-particle partitioning into bins of different particle sizes, as well as condensed-phase chemistry and diffusion in each particle size bin over time. The results are compared with previous modelling efforts that did not explicitly treat NPF and assumed a single, effective particle size [2,3]. We demonstrate the capability of the newly developed model to describe the experimental data. We find that particle-phase chemistry and diffusion have pronounced effects on the formation and evaporation rate of SOA. We investigate the effect of oligomerization and phase state on mass growth and evolution of size distribution. We explore how nanoparticle growth rates are affected by these processes.

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## Breakdown of the Stokes-Einstein relation in Stillinger-Weber silicon

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Topic: Multiscale Methods

We investigate the dynamical properties of liquid and supercooled liquid silicon, modeled using the Stillinger-Weber (SW) potential, to examine the validity of the Stokes-Einstein (SE) relation. Towards this end, we examine the relationship among various dynamical quantities, including (i) the macroscopic transport coefficients - self diffusion coefficient $D$ and viscosity $\eta$, (ii) relaxation time $\tau_\alpha$ as well as (iii) lengthscale dependent relaxation times $\tau_\alpha(q)$ over a broad range of temperature $T$, pressure $P$ and density $\rho$ covering both equilibrium and metastable liquid state points in the phase diagram. Our study shows a weak break down in SE relation involving $D$ and $\eta$, and the loci of the breakdown of the SE relation (SEB) is found in the high T liquid phase. The $\tau_\alpha$, when used as a proxy to $\eta$, shows distinct breakdown in the SE relation whose loci is found in the supercooled liquid phase. Interestingly, certain parts of the phase diagram shows that loci of onset of slow dynamics lie below the loci of SEB, suggesting a regime that exhibits Arrhenius but non-Fickian behaviour. Computation of $\tau_\alpha(q)$ enables us to extract the lengthscale associated with the Fickian to non-Fickian behaviour using which we show that the breakdown of the SE relation occurs only below a specific lengthscale at a given temperature. Further we also compare the SEB loci with other features of the phase behaviour, including the loci of compressiblity maximum, density maximum as well as diffusivity maximum. [1]

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# Parameter Sensitivity Analysis of Plate Motion using the Adjoint Method and Automatic Differentiation

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Topic: Interdisciplinary Applications, Uncertainty Quantification & Inverse Methods

The adjoint method for the Stokes equations provides a versatile and highly efficient approach to investigate the underlying physics of geodynamic processes. Reuber et al. [1] demonstrated that adjoint sensitivities can be used to develop scaling laws for processes like folding and subduction dynamics. The gradients derived using the adjoint method can also directly be used in inversions in geodynamic applications. However, previous implementations of the adjoint method have typically been highly problem-dependent and often limited to viscous rheologies. Extending it to other nonlinear rheologies typically required substantial additional work, which is likely one of the reasons that the method has not yet been widely adopted in solid Earth geosciences. To overcome this problem, we use automatic differentiation (AD) to compute the gradients needed to develop an adjoint solver for the Stokes equations. The gradients are computed using the Julia package Enzyme.jl. The adjoint solver is designed to be problem-agnostic, where the gradients are automatically computed for any user-defined rheology, from a simple linear viscous model to a complex visco-elasto-viscoplastic composite rheology. This functionality is added to the JustRelax.jl thermo-mechanical solver, where we use the same pseudo-transient solver strategy to solve both the forward and adjoint problems. This approach ensures that the adjoint solver remains consistent and fully generic. The method is applied to analyse horizontal plate motion around subduction zones. For different material parameters, it is possible to calculate sensitivity kernels that show, for each location in the numerical domain, how much these parameters influence the horizontal plate motion (e.g. [2]). The scaling of sensitivities for different parameters is discussed to enable a quantitative comparison. This approach is then used to identify the most influential factors affecting plate motion.

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## A path integral approach to cloud modeling

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Topic: Stochastic Models

In large-scale, physics-driven weather and atmospheric models, clouds are conventionally represented as sets of differential equations, where particles are either integrated into moment-based schemes or aggregated into larger super-particles. However, these approaches inherently lack the capacity to capture both the discrete nature of particle-based processes in clouds (e.g., nucleation, evaporation) and the intrinsic stochastic influences on these processes [1]. This study introduces a novel approach to incorporate these critical aspects of cloud-internal processes into a path integral description of a single cloud cell. By synergistically combining the established Doi-Peliti and Martin-Siggia-Rose response field formalisms [2], our framework enables the concurrent treatment of stochastically modeled particles (ice crystals) and a deterministic background field with a stochastic noise component (saturation). Leveraging this integrated approach, we can efficiently compute expected averages of cloud states (encompassing both particles and saturation) and intrinsic fluctuations, obviating the need for computationally intensive relaxation processes. This capability is demonstrated through an exemplary application to a simplified cloud cell, incorporating nucleation, sedimentation, and updraft processes.

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## Numerical modeling of simultaneous diffusion and mineral growth

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Topic: Interdisciplinary Applications

Compositional concentration profiles across individual crystals or diffusion couples are largely determined by diffusion and growth processes. These two processes are particularly important during the formation of high-temperature rocks such as igneous and metamorphic rocks. The numerical simulation of concentration profiles in crystals is a widely used technique in various fields such as geospeedometry or diffusion chronometry. Compared to single crystals, coupled diffusion pairs yield tighter constraints on the experienced temperature and pressure ranges and thus provide additional information for our models. However, the numerical description of concentration profiles within diffusion couples is challenging due to the sharp compositional gradients. Discontinuities in concentration, which are related to the different mineral properties, commonly occur at the interface of two minerals and lead to technical implementation issues. To address these issues, we have developed a Finite Element (FE) package in Julia that can calculate the evolution of concentration profiles in diffusion couples with moving interfaces. Both growth and diffusion processes are considered. An adaptive grid enables the accurate reproduction of rapid concentration changes and discontinuities. Our code can be applied to various examples of single crystals or diffusion couples, integrating any combination of growth, diffusion, and temperature dependency. Additionally, it is possible to calculate concentration profiles based on the thermodynamically-constrained, Stefan-Interface condition. Results from our models can be used in petrology and geodynamic applications to provide tighter constraints concerning in the pressure and temperature evolution of magmatic and metamorphic mineral assemblages.

## Solutions of the population balance equation of cloud hydrometeors

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Topic: Multiscale Methods

Clouds constitute an ensemble of a huge number of particles. A general approach for representing the system is the use of size or mass distributions, leading to a population balancing equation (PBE). Since solving this equation is quite challenging and computationally expensive, numerical weather prediction (NWP) models often use so-called bulk schemes, based on general moments of the underlying distribution, and assuming a fixed functional form for the particle size distribution, from which evolution equations for the moments are derived. These schemes are much simpler and computationally cheap, however introducing conceptual issues.
In this work, we directly address the problem of solving the PBE for the mass distribution of atmospheric hydrometeors. We derive an analytical solution in a simplified scenario where both the hydrometeor mass growth rate and terminal fall speed follow power-law dependencies on mass. Additionally, the supersaturation and the air density profile are assumed constant. The analytical solution sets a benchmark for future numerical studies on which the interactions are further refined.
For the case on which only diffusional growth is considered an analytical solution is found for the time evolution of the number and mass concentration. The contribution to the evaporation of the number concentration is determined via the integrable singularity present in the distribution function [2]. In the growth regime, our current results coincide with those predicted by the classic two moment bulk scheme, obtaining the same power laws. However, when evaporation regime is considered, the dynamics seem to differ considerably from the power laws predicted by the bulk scheme.

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## Reconstructing, Predicting and Understanding Cloud Structure Formations

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Topic: HPC & Machine Learning, Interdisciplinary Applications

Modeling the microphysics of cloud structures poses a significant challenge to in current atmospheric models due to the vast range of temporal and spatial scales involved. Achieving a better understanding of the underlying physical processes is a main goal in cloud physics.
In this study, we approach the problem from an information-theoretic perspective, guided by three key questions: (1) To what extent can coarse-scale atmospheric data be used to reconstruct the appearance of cloud fields? (2) How far into the future can current atmospheric conditions reliably predict cloud structures, and what are the limits of such predictability? (3) Can deep learning models help uncover meaningful insights into the physical mechanisms that govern cloud formation?
We use ERA5 reanalysis data, which probably provides the best description of the atmospheric state available. We use this data as input to a regressor based on deep neural networks, trained to reproduce satellite observations from two orbiting NASA satellites. We obtain estimates that are more accurate than the optical thickness calculated from ERA5, demonstrating that significant information about cloud structures is embedded in the atmospheric state and can be extracted using purely data-driven methods.
We extend our investigations to examine the temporal generalization of these models across varying climatic regions. Thereby, predictive power varies from approximately 24 up to 96 hours, depending on the atmospheric stability. Additional experiments with reduced inputs show that even when key physical quantities are withheld, prediction quality often remains high. This suggests that predictive information is redundantly encoded across the data, supporting an information-theoretic interpretation of cloud formation as a distributed process.
Since neural networks only implicitly describe highly complex functions, gaining insights into the underlying processes is quite difficult. We apply gradient-based saliency methods to examine the model's behavior. Initial results reveal anecdotal evidence suggesting that different factors dominate in different regions. However, surface temperature and the atmospheric water content play a particularly important role. For a larger time horizon, water transport appears to be essential.
Our study demonstrates that it is possible to reconstruct and predict cloud structures from atmospheric conditions using neural networks. While the intrinsic complexity of these models prevents an explicit formulation of the underlying relationship, gradient-based analyses provide some hints concerning the dominant physical drivers, which might help improving our understanding of atmospheric dynamics.

## Numba-MPI & PyMPDATA: JIT-compilation and multi-threading for high performance computing in Python

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Topic: HPC & Machine Learning

Numba-MPI [1] is a pure Python package providing wrappers for MPI (Message Parsing Interface) C API that can be used from Numba JIT (Just In Time)-compiled code. This allows computational tasks to benefit from multi-threading, JIT-compilation and workload scaling on multi-node computer clusters. JIT compilation provides a way of achieving compiled-code performance using pure-Python codebase, requiring no prior compilation or linking (both of which are triggered automatically on a first call to a given function). The package is developed targeting compatibility across Linux, Windows and macOS, and OpenMPI, MSMPI, MPICH and Intel MPI implementations, all of which is ensured via continuous integration workflows. The package enables interoperability with higher-level mpi4py MPI interface (outside of JIT-compiled code blocks). Numba-MPI implements both synchronous and asynchronous communication functions from MPI C API.

Numba-MPI is a dependency of two Python packages for numerically solving PDEs: py-pde [2] and PyMPDATA [3], the latter providing JIT-compiled implementation of the Multidimensional Positive Definite Advection Transport Algorithm (MPDATA) for solving advection-diffusion problems. PyMPDATA features hybrid multi-threading and MPI-based domain-decomposition parallelism. On the one hand, the package constitutes a reusable building block for development of advection-diffusion simulation solvers. On the other hand, the package ships with ready-to-use examples, maintained in a form of Jupyter notebooks, and covering solutions of such problems as Burgers, Black-Scholes, Boussinesq and shallow-water equations. In the poster, I will outline the features, architecture and usage examples of Numba-MPI coupled with PyMPDATA. Both packages are open source and collaboratively developed on GitHub, with maintenance led by our group at the AGH University of Krakow.

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## Deep learning-based generation of 3D cloud structures from geostationary satellite data

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Topic: Interdisciplinary Applications, Multiscale Methods

The Nanoscale Theory and Modeling team is one of current five research groups within the newly established Aerosol Chemistry Department at the Max Planck Institute for Chemistry. The team focuses on molecular- and nanoscale-level modeling of atmospheric aerosol formation, degradation, and transport. Aerosol particles form and grow ubiquitously throughout Earth's atmosphere, impacting quality of life in multiple ways. They influence climate by serving as cloud condensation nuclei (CCN), and affect regional and global air quality through the formation of particulate matter (PM). Normally, aerosol formation involves three major stages, distinguished by the chemical species involved and their associated physicochemical processes (see Fig. 1): (1) the oxidation of precursors emitted from biogenic and anthropogenic sources, (2) the nucleation of oxidation products to form stable nuclei, and (3) the subsequent growth of these nuclei into larger particles capable of influencing climate. Due to the complexity and diversity of species and processes involved, the detailed mechanisms governing atmospheric aerosol formation remain poorly understood. In this presentation, we will begin by introducing the research aims and topics of the newly established Nanoscale Theory and Modeling team, with particular emphasis on its recent focus on the phenomenon of atmospheric aerosol formation. We will then highlight several of our recent modeling studies that investigate the molecular- and nanoscale-level mechanisms underlying the formation and growth of aerosol particles in the atmosphere2-5.

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## Aerosol-Cloud-Precipitation Interactions: Insights from Radar Observations and Model Simulations

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Topic: HPC & Machine Learning

Atmospheric aerosols influence cloud systems and precipitation through complex processes, yet their effects on convection and mesoscale convective systems (MCSs) remain poorly understood. In particular, how aerosols alter interactions between MCSs and their ambient environment, thereby affecting MCS climatology, is still unclear. This study examines the climatology of mature MCSs and their interactions with anthropogenic aerosols over South China during spring (March to May) from 2009 to 2019 by combined observations and model simulations. An independently developed algorithm was employed for objective diagnosis of radar reflectivity data, revealing that most MCSs exhibited linear or quasi-linear structures, with convective precipitation constituting approximately 34% of the precipitating area and 63% featuring trailing stratiform precipitation. Diurnal cycles shifted from midday peaks in March to nocturnal peaks in April and May. A significant inverse correlation between aerosol pollution days and MCS occurrences was observed in April during 2013-2019. In contrast, the correlations between surface PM abundance and MCS frequency varied across different months, reflecting seasonal modulation by regional dynamic and thermodynamic conditions. Model simulations further indicated that elevated anthropogenic aerosol levels reduce April MCS occurrences by 21%-32%, leading to decreased precipitation. This suppression is driven equally by aerosol-induced radiative stabilization of the atmosphere and by microphysical and dynamical changes within MCSs. Our results demonstrate the complex effects of aerosols on MCSs through their impacts on both the convective systems themselves and the surrounding regional atmosphere.

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## Environmental and health impacts of urban residential energy switching in China

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Topic: HPC & Machine Learning

Exposure to air pollution by burning solid fuels (such as coal) for residential cooking and heating in China has caused significant health impacts in the past. The government has implemented measures to replace coal with relatively clean energy sources (e.g., natural gas). However, the scale and scope of health benefits associated with such energy switching in an urban context, when considering both ambient and indoor air quality, remain unclear. Here we used an atmospheric chemical transport model showing that relatively clean energy use increased from 2% to 71% from 1980 to 2014, and although annual premature deaths attributed to particulate matter with an aerodynamic diameter less than 2.5 $\mu$m (PM2.5) from urban residential sources increased from 136,000 (87,000–194,000) to 202,000 (117,000–302,000) during the same period, this was primarily due to population growth, urbanization, aging, and background mortality rate changes. In the absence of energy switching, there would have been 2.2 million additional premature deaths. The results provide solid evidence on health benefits of energy switching, suggesting further switching to cleaner energy for expanded health-climate co-benefits. In the future, we aim to incorporate machine learning as a tool to further improve the datasets and the modeling processes employed in this study.

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