SCCS 2017

Scaling Cascades in Complex Systems

CRC 1114

Abstracts

CRC 1114 Conference 2017
Scaling Cascades in Complex Systems

	Monday, March 27		Tuesday, March 28		Wednesday, March 29	
07:30–08:30	Registration					
08:30	Welcoming speech by Brigitta Schütt, Vice President of Freie Universität Berlin					
08:30–09:30	Keynote Rupert Klein		Keynote Taras Gerya		Keynote Mark Peletier	
09:30–10:30	Keynote Carsten Eden		Keynote Michael Dellnitz		Keynote Gary Froyland	
10:30–11:00	Coffee break		Coffee break		Coffee break	
11:00–13:00	Mini Symposium *Balanced atmospheric data assimilation*	*Organization, shape, and dynamics of biological membranes*	Mini Symposium *Practical approximations for Monte Carlo simulations of complex systems*	*Deformation accumulation in seismic faults and networks*	Mini Symposium *Open systems*	*Molecular kinetics and kinetic models from MD simulations*
13:00–14:30	Lunch break		Lunch break		Lunch break	
14:30–16:30	Mini Symposium *Information-theoretical methods for complex systems*	*Multiscale methods for PDEs: Methodology and applications*	Mini Symposium *Stochastic parametrizations for convective processes*	*Coarse graining in molecular systems*	Mini Symposium *Stochastic modeling approaches for turbulent flows*	*Multi-scale reaction kinetics*
16:30–17:00	Coffee break		Coffee break		Coffee break	
17:00–18:00	Keynote Robert Scheichl		Keynote Mária Lukáčová-Medvid'ová			
18:00	Icebreakers and Poster Session				Closing words	
19:00			Conference Dinner			

KEYNOTES

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Carsten Eden

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Robert Scheichl

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Vladimir Kazeev

Tensor product decomposition methods applied to multi-scale data with self-similar characteristics
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Recent advances in tensor numerical methods for multi-dimensional PDEs
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An embedded corrector problem for stochastic homogenization
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The apparent weakness of active faults
Jean Paul Ampuero

An integrated view of earthquake source dynamics associated with the 1992 Landers earthquake and the 2004 Sumatra megathrust earthquake
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Rate-and-state friction: From analysis to simulation
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Robert Plant

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Stochastic chaos in a turbulent von Karman flow
Davide Faranda, Yuzuru Sato, Brice Saint-Michel, Berengere Dubrulle and Francois Daviaud

Flow regimes and scale interactions in the stably stratified atmospheric boundary layer
Nikki Vercauteren

Beyond the limit of infinite time-scale separation: Edgeworth approximations and homogenisation
Jeroen Wouters

Energy conserving stochastic models of the atmosphere
Christian L. E. Franzke and Federica Gugole

Optimisation of an idealised primitive equation ocean model using stochastic parameterization
Fenwick Cooper

Multi–scale reaction kinetics

Combining molecular dynamics with mesoscopic Green's function reaction dynamics simulations
Pieter Rein ten Wolde

Move before reacting – multi-scale motion of molecules in biological/bio-mimetic fluids
Matthias Weiss

The spatiotemporal chemical master equation
Stefanie Winkelmann

Collaborative Research Center (CRC) 1114
Scaling Cascades in Complex Systems: Across-scale modelling and simulation paradigms

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Funded by Deutsche Forschungsgemeinschaft (DFG) and hosted by Freie Universität Berlin, CRC 1114 has been in operation since October 2014. Colleagues from the university's Biology/Chemistry/Pharmacy, Physics, Geo-Sciences, and Mathematics & Informatics departments join forces in this program with partners from Technical University of Berlin, and Potsdam University, from the Helmholtz Society's Geo-Research Center Potsdam, the Max Planck-Institute for Colloids and Interfaces, the Leibniz-Association's Weierstraß Institute for Applied Analysis and Statistics, and from Zuse-Institute Berlin.

The center's goals originate from the observation that the majority of rigorous mathematical results on "multi-scale problems" actually involve merely *two*, typically separated, scales, whereas there is a myriad of phenomena studied in the applied sciences that involve *many*, in the sense of (many) more than two, and not necessarily separated, scales. As a result, a variety of modelling and simulation approaches has been developed to address the specific needs of individual applications. An overarching framework, however, that would allow for a systematization and classification of (truly) multi-scale problems from a mathematical perspective and that would facilitate the cross-fertilization of ideas between disciplines and application fields is missing as yet.

This CRC aims at developing the foundations of such a framework. Its individual projects are motivated by challenging applied-science problems from the bio-, geo-, and material sciences that feature some type of "cascade of scales". The projects aim to make substantial progress on the application side while jointly contributing, over the program's 12-year lifetime, to the development of generalizable "across-scale modelling and simulation paradigms". This presentation will highlight some of their recent achievements and discuss them in the light of the program's overarching scope.

The energy cycle and ocean model parameterisations

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The energy transfers between the three principal dynamical regimes – small-scale turbulence, internal gravity waves and geostrophically balanced motion – are fundamental to the energy cycle of both the atmosphere and the ocean. Nonetheless, they are poorly understood and quantified, and their representation in state-of-the-art Earth system models is unsatisfactory. Since the interactions of the dynamical regimes ultimately link the smallest scales to the largest scales by a variety of complex processes, understanding these interactions is mandatory to construct atmosphere and ocean models and to predict climate. The current lack of understanding is reflected by energetically inconsistent models with relatively large biases, but also paralleled by inconsistencies of a numerical and mathematical nature. The recently established SFB/TRR 181 aims to combine recent efforts to overcome these deficiencies, to foster new activities to understand the dynamical interactions, and to improve the consistency of ocean and atmosphere models.

Central to the concept of energetic consistency is IDEMIX, a model for propagation, refraction and dissipation of internal gravity waves in the ocean. The concept will be explained and applied to predict forcing of the mean flow by breaking waves in the ocean, and gravity wave drag by interaction with sheared mean flow. The concept will also be applied to predict Rossby wave drag on the mean flow – which is identical to baroclinic instability – to parameterized the effect of unresolved geostrophic eddies in ocean models.

Multilevel Monte Carlo and beyond

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Multilevel Monte Carlo (MLMC) is a recently introduced variance reduction technique for stochastic simulation which greatly reduces the computational cost by employing cheap, coarse-scale models with lower fidelity to carry out the bulk of the stochastic simulations, while maintaining the overall accuracy of the fine scale model through a small number of well-chosen high fidelity simulations.

In this talk, I will first review the ideas behind the approach and discuss a number of applications and extensions that illustrate the generality of the approach. The multilevel Monte Carlo method (in its practical form) has originally been introduced about 10 years ago by Mike Giles for stochastic differential equations in Mathematical Finance and has attracted a lot of interest in the context of uncertainty quantification of physical systems modelled by PDEs. (The first, theoretical paper was by Stefan Heinrich in 1998.) The approach has been extended to Markov chain Monte Carlo, sequential Monte Carlo and other filtering techniques. Among others, its application has been extended to biological/chemical reaction networks, plasma physics, interacting particle systems and more recently to nested simulations.

In the second half of the talk, I will go beyond the classical MLMC framework and use sample-dependent model hierarchies and a posteriori error estimators to efficiently estimate rare events (*Multilevel Subset Simulation*) as well as to extend the framework from the discrete, level-based approach to a new *Continuous Level Monte Carlo (CLMC)* method. These latter extensions are work in progress in collaboration with Gianluca Detommaso (Bath), Tim Dodwell (Exeter) and Daniel Elfverson (Umeå).

Multi-scale modeling of geological and technological processes with marker in cell techniques

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Numerical modeling of geological and technological processes is an essential approach in both science and industry with ever-growing demand and high efficiency/cost ratio. Current trend in science is to develop universal approaches with potentially unlimited number of applications. Here, I present a simple and flexible method based on staggered finite differences and marker in cell techniques (e.g., [1]), which demonstrated superior performance in several branches of modern quantitative Earth sciences. It is suitable for modeling various long-term and short-term thermomechanical processes involving large 3D deformation of rheologically complex materials. Recently, potential applicability of this method to technological processes (material science) and natural processes of industrial significance (geo-hydro-mechanics, waste deposits) has also been demonstrated. This presentation gives a short theory of the method and discuses modeling examples of natural and technological significance.

[1] T. Gerya. *Introduction to Numerical Geodynamic Modelling.* Cambridge University Press, 345 pp., 2010.

Glimpse of the infinite – the approximation of invariant sets for delay and partial differential equations

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In this talk we present a novel numerical framework for the computation of finite dimensional invariant sets for infinite dimensional dynamical systems [1]. With this framework we extend classical set oriented numerical schemes (for the computation of such objects in finite dimensions) to the infinite dimensional context. The underlying idea is to utilize appropriate *embedding techniques* for the reconstruction of invariant sets in a certain finite dimensional space. Finally, we illustrate our approach by the computation of attractors both for delay and for partial differential equations.

[1] M. Dellnitz, M. H. Molo, and A. Ziessler. On the computation of attractors for delay differential equations. *Journal of Computational Dynamics*, 3(1):93–112, 2016.

How to bridge large scale differences?

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In this contribution we present two examples of modeling multiscale problems such as the polymer-solvent mixtures and colloid-polymer systems. Of course, the most accurate description of such complex soft matter systems would be obtained by the molecular dynamics (MD). However, such miscroscale model is computationally inefficient if large scale regions in space and time need to be simulated. We present two approaches how to overcome this restriction and to obtain practically tractable simulation techniques to bridge macroscopic and microscopic models.

Firstly, we present a new *reduced-order hybrid multiscale method* that is based on the combination of the discontinuous Galekin method and molecular dynamics simulations, see [1]. We follow here the framework of the heterogeneous multiscale method that makes use of the scale separation into macro- and micro-levels. On the macro-level the governing equations of the incompressible flow are the continuity and momentum equations. The equations are solved using a high-order accurate discontinuous Galerkin method. The missing information on the macro-level is represented by the unknown stress tensor that is evaluated by means of the molecular dynamics simulations on the micro-level.

The data obtained from the MD simulations underlie relatively large stochastic errors that can be controlled by means of the least-square approximation. Moreover, in order to reduce a large number of computationally expensive MD runs we use the reduced order approach. We split the computations into an off-line phase of expensive training and an on-line phase of fast multiple queries. In the training phase we use the Greedy sampling algorithm as a model reduction technique to replace the unknown nonlinear stress-strain function by a reliable low-dimensional approximation. Numerical experiments confirm the robustness of our newly developed hybrid MD-dG method.

In the second part of our presentation we present a new second order *energy dissipative finite volume-finite difference scheme* to treat macroscopic equations aiming at the modeling of the dynamics of complex polymer-solvent mixtures. This model consists of the Cahn–Hilliard equation for diffuse interface phase fields and the Oldroyd-B equations for the hydrodynamics of the polymeric mixture, cf. [2]. A complementary approach to study the same physical system is realized by simulations of a microscopic model based on a hybrid Lattice Boltzmann-MD scheme. These latter simulations provide initial conditions for the numerical solution of the macroscopic equations. Our ultimate goal is the systematic coarse-graining of simulation models by means of optimal control of well-chosen observables, such as structure factors.

The present research has been supported by the German Science Foundation under the grant TRR 146 "Multiscale Simulation Methods for Soft Matter Systems."

[1] N. Emamy, M. Lukáčová-Medvid'ová, S. Stalter, P. Virnau, and L. Yelash. Reduced-order hybrid multiscale method combining the Molecular Dynamics and the Discontinuous-Galerkin method, 2017. submitted.
[2] M. Lukáčová-Medvid'ová, B. Dünweg, P. Strasser, and N. Tretyakov. Energy-stable numerical schemes for multiscale simulations of polymer-solvent mixtures, 2017. submitted.

Upscaling the dynamics of dislocations

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Plasticity, the permanent deformation that one observes in metals, is the net effect of the movement of a large number of microscopic defects in the atomic lattice. These defects, called dislocations, are curve-like topological mismatches, and migrate through the metal under the influence of internal and external forces. Macroscopic, permanent, deformation arises through the concerted movement of a large number of these dislocations.

It is a major challenge to connect a microscopic description of dislocation movement on one hand with models of macroscopic plastic behaviour on the other hand. If this were possible, then much could be gained: metals could be designed at the workstation with tailor-made properties, design of hybrid materials would become much easier, and generally the holy grail of 'materials by design' would come a little closer. At this stage we are not able to do this; there is a major gap between the models at these different spatial and temporal scales. Part of the difficulty lies in the complex interactions between dislocations: they attract and repel each other, and form complex higher-level structures that appear to play an important role in determining the macroscopic behaviour.

Interestingly, the situation for the dynamics of the dislocations is significantly more complex than that of the energetics.

I will outline some recent results in this field, describe some of our own recent results in two dimensions, and mention some open questions and one or two mysteries.

This is joint work with Adriana Garroni, Marc Geers, Markus Hütter, Patrick van Meurs, Ron Peerlings, and Lucia Scardia.

Coherence and multiscale dynamics in geophysical flows

Gary Froyland
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Oceanic and atmospheric dynamics operate over a wide variety of timescales. Certain "coherent" features such as oceanic eddies and gyres and atmospheric vortices survive over timescales much longer than surrounding fluid regions. These coherent objects play an important role in the transport of heat, salt, carbon, and nutrients in the ocean, and strongly affect weather systems in the atmosphere. I will discuss a variety of techniques for extracting these objects from models and observational data.

Mini Symposium

Balanced atmospheric data assimilation

Monday, March 27
Lecture Hall, ZIB

Organizers
Gottfried Hastermann, Rupert Klein, Sebastian Reich

Chair
Sebastian Reich

The atmosphere's multi-scale structure poses several major challenges in numerical weather prediction. One of these arises in the context of data assimilation. The large scale dynamics of the atmosphere is balanced in the sense that acoustic or rapid internal wave oscillations generally come with negligibly small amplitudes. If triggered artificially, however, through inappropriate initialization or in the course of data assimilation, such oscillations can have a detrimental effect on forecast quality as they interact with the moist aerothermodynamics of the atmosphere. The aim of this minisymposium is to discuss this issue from two different perspectives. First we will discuss extensions of existing assimilation strategies to avoid the artificial fast scale dynamics, secondly we will consider the problem from a model perspective, since multi-scale numerical methods may also provide an answer to the balancing problem.

Speakers

11:00 AM	Nils Wedi
11:30 AM	Stefanie Hollborn
12:00 PM	Tommaso Benacchio
12:30 PM	Maria Reinhardt

Multi-scale characteristics of ECMWF's assimilation and forecast system

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Numerical weather prediction (NWP) is dominated by the sensitivity of the governing equations to the initial conditions. This leads to the data assimilation problem of deriving the state of the atmosphere by optimally mapping billions of observations to the numerical model grid (with equally billions of gridpoints), while at the same time satisfying fundamental balances forming a subset of the governing equations. If not, unrealistic, high frequency oscillations are the result, arising particularly from imbalances in connecting the mass (temperature, surface pressure and geopotential) and the wind field (divergence, vorticity). In data assimilation, it is primarily the background error covariance matrix that determines how information from observations spreads to nearby gridpoints and to vertical levels of the assimilating model, and determines in particular how observations of the wind field are used to extract information from the mass field and vice versa [1]. Since sampling background error invariably requires the true atmospheric state which we don't have at gridpoint locations, a model is employed with statistical properties (hopefully) similar to the unknown background error. It is this background error covariance model that closely links analytical models of known dynamical balances, statistical relationships between variables, spatial and temporal filtering, and the application of multiscale numerical methods to represent spatially and temporally varying background error statistics [1]. At ECMWF the latter are derived from an ensemble of suitably perturbed 4dvar data assimilations [2]. The talk will describe selected multi-scale characteristics of ECMWF's forecast [3] and assimilation system and discusses potential improvements required in order to benefit from increased horizontal resolution with complex topography and permitted convection.

[1] M. Fisher. Background error covariance modelling. *Proc. ECMWF Seminar on Recent Developments in Data Assimilation for Atmosphere and Ocean, Reading, UK*, pages 45–64, 2003.
[2] E. H. M. Bonavita, L. Isaksen. On the use of EDA background error variances in the ECMWF 4D-Var. *Tech. Memorandum, Reading, UK*, 664:1–30, 2012.
[3] S. Malardel and N. Wedi. How does subgrid-scale parametrization influence nonlinear spectral energy fluxes in global NWP models? *J. Geophys. Res. Atmos.*, 121:5395–5410, 2016.

The multi-scale data assimilation system at the German Meteorological Service

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Weather happens at extremely varying time and space scales, from seasonal weather conditions ranging over weeks and continents to rapidly changing high impact weather such as thunderstorms and strong precipitation that are often most hazardous only in small areas. Based on the ubiquitous influence of weather on personal life as well as on society it is of great importance to steadily improve numerical weather prediction by refining models and assimilation techniques, by increasing resolution, by including and exploiting more observations, and by enhancing stability and reliability. The agenda of weather and climate forecasting and projection today includes the development and operation of ensemble forecasting system (EPS) on all scales, which have the ability to model and describe the distribution of possible events and as such the variability of extreme weather, its variables and phenomena. We describe the setup of the ensemble data assimilation (EDA) and forecasting systems which have been developed and are under development at German Meteorological Service (DWD), thereby paying particular attention to the methods used in order to comply with balance laws. The presentation comprises the ICON global model with its hybrid ensemble variational data assimilation (EnVAR) and ensemble prediction system ICON EPS as well as the high-resolution ensemble data assimilation system COSMO-KENDA (Kilometer Scale Ensemble Data Assimilation), which has only recently been introduced as the regional operational system at DWD.

A blended semi-implicit numerical model for multiscale atmospheric flows and balanced data assimilation

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Atmospheric flows develop across a wide range of spatial and temporal scales. Fast waves associated to compressibility and buoyancy are generally deemed insignificant for most weather-relevant low Mach number flows, yet they force fully elastic numerical models to run with inefficiently small time steps. In data assimilation, spurious waves arising from acoustically imbalanced data can quickly spread across the domain and severely affect forecast skill. Reduced soundproof formulations such as the anelastic and pseudo-incompressible models, traditionally applied on small and meso-scales, constrain the flow divergence and suppress acoustics at the outset. On the other hand, hydrostatic primitive models free of vertically propagating acoustics suit well efficient simulations of synoptic and planetary flows.

A blended numerical strategy is presented, whereby a semi-implicit fully compressible formulation asymptotes to pseudo-incompressible dynamics for small scales and low Mach number and efficiently operates with a time step limitation independent of sound speed. The second-order accurate conservative discretization features an explicit predictor followed by two elliptic solvers for the correction of advecting fluxes and momentum. Compressibility is encoded on a switch in the mass-weighted temperature equation and amounts to the addition of a zero-order term Helmholtz term to the Poisson elliptic problems of the soundproof case. Progress towards buoyancy-implicit numerics will also be discussed and preliminary results shown. Warm air bubble runs highlight the reduction of acoustic imbalance achieved by operating the model in soundproof mode for a few spinup time steps after which the discretization is smoothly switched to full compressible dynamics. Extended to a recently developed doubly-blended analytical formulation able to access hydrostatic as well as pseudo-incompressible dynamics, the strategy can be employed as a general tool to filter out unwanted spurious perturbations from assimilated data in compressible runs across scales.

Preserving balance in data assimilation

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Data Assimilation (DA) is the bridging between data produced by a physical model and data obtained by observing a signal. Both data sets are incomplete and prone to errors and the goal of DA is to estimate the probability distribution

$$\pi(\text{model state}|\text{observations}).$$

One way to do so is sequential filtering, where one alternates between forwarding the model for n time steps, obtaining the forecast and then applying a filter algorithm to include the information about available observations, obtaining the analysis.

We are working on Data Assimialation techniques in the context of dynamical systems with multiple scales like e.g.

$$\dot{X} = F(X, Y)$$
$$\varepsilon^2 \dot{Y} = G(X, Y)$$

where the small ε causes $Y \in \mathbb{R}^{N_y}$ to evolve on a much shorter time scale than $X \in \mathbb{R}^{N_x}$. The subset $\mathcal{M} \subset \mathbb{R}^{N_x} \times \mathbb{R}^{N_y}$ of phase space defined by $(x, y) \in \mathcal{M}$ iff $G(x, y) = 0$ is formally called a slow manifold. Smooth solutions have to satisfy

$$G\big(X(t), Y(t)\big) = \mathcal{O}(\varepsilon^2). \tag{1}$$

We refer to a model state $\big(X(t), Y(t)\big)$ which satisfies equation (1) as balanced.

DA alogrithms can destroy balance relations because of the intermittent nature of how observations are integrated in sequential DA and also because of localization, which is an essential tool to make DA work in practice. The violation of balance leads to high frequency oscillations and ultimately to unphysical predictions.

In this talk we present two strategies for producing balanced analysis fields. The first one is to calculate the analysis field on a coarser subgrid followed by an interpolation step onto the actual computational grid which preserves the balance. This is achieved by formulating the interpolation step as a minimisation problem including a penalty term with respect to the balancing relation residual.

The second approach on the other hand focuses on the forecasting part: a modified time stepping method is used as a time discretisation for the model. In the first time step after the assimilation procedure, the model state is projected onto the slow manifold and for a few following steps the time stepping method blends towards an energy preserving time discretization of the full model.

Mini Symposium

Organization, shape, and dynamics of biological membranes

Monday, March 27
Lecture Hall, Informatik

Organizers
Carsten Hartmann, Ralf Kornhuber, Frank Noé, Christof Schütte, Thomas Weik

Chair
Ralf Kornhuber

The morphology and molecular organization of biological membranes is resulting from the interplay of a diversity of processes on multiple temporal and spatial scales. Typical modelling approaches involve and sometimes combine molecular dynamics and coupled systems of geometrical pdes. This minisymposium is devoted to the computational modelling of the organization, shape, and dynamics of biological membranes by chemical and mechanical interaction of proteins in bilipid layers.

	Speakers
11:00 AM	Christoph Haselwandter
11:30 AM	Carsten Gräser
12:00 PM	Mohsen Sadeghi
12:30 PM	Michael Kozlov

Assembly, shape, and stochastic dynamics of membrane protein lattices

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Cell membranes are one of the fundamental hallmarks of life. Following seminal breakthroughs in structural biology and cell microscopy, it is now widely appreciated that many of the key aspects of membrane function cannot be understood by considering isolated membrane proteins but, instead, emerge from the collective properties of protein structure, interactions between proteins and the surrounding lipid bilayer, membrane shape, and the supramolecular organization of membrane proteins into lattices of interacting proteins. Using specific biological model systems as case studies, we show here how experimental data on the structure, organization, dynamics, shape, and collective function of cell membranes can be integrated into multiscale mathematical models that allow, starting from key molecular properties of proteins and lipids, a physical understanding of cell membranes across length and time scales.

Modeling and simulation of particles in membranes

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A variety of models for the membrane-mediated interaction of particles in lipid membranes are considered in the literature. We present a mathematically consistent variational framework for the mathematical treatment of models for particle membrane coupling. Based on this framework we derive numerical methods for the simulation of particles in membranes. In order to efficiently treat moving particles driven by mechanical interactions the presented methods combine ideas from shape optimization and fictitious domain finite elements.

Coarse-grained membrane model for mesoscopic simulation of cellular dynamics

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We present a simple and computationally efficient coarse-grained model for simulating lipid bilayer membranes. This solvent-free model consists of a double layer of representative particles, with bond-stretching and angle-bending interactions amongst nearest neighbors. A semi-analytical scheme is used for parameter space optimization of interaction potentials, with the aim for the model to best reproduce the Canham-Helfrich energy density over a range of relevant curvatures. Furthermore, in-plane fluidity is implemented with Monte Carlo bond-flipping moves. In order to verify the applicability of the model, three sets of computer experiments are performed. First, tensionless membrane patches are equilibrated and their thermal undulation spectrum is analyzed to recover the input bending stiffness against which the potential parameters are optimized. Second, shear flow under a gravity-like force is simulated to calculate the effective viscosity manifested by bond-flipping moves. And third, interaction of the bilayer membrane with a spherical nanoparticle is simulated as a test case for large membrane deformations involved in cellular processes such as endocytosis. The results are shown to coincide well with the predicted behavior of continuum models. Ultimately, we aim to employ this coarse-grained membrane model in particle-based reaction-diffusion simulations to study cellular signal transduction.

Modeling lipid droplets on membrane tubules

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Membrane tubules of few tens of nanometer cross-sectional diameters and micron-scale lengths represent a basic structural component of intra-cellular organelles, such as endoplasmic reticulum and Golgi Complex, and emerge from plasma membranes in the course of cell crawling on extra-cellular matrices and substrates. Besides barrier functions, the tubular membranes serve as platforms for formation of peculiar cell organelles, Lipid Droplets and Migrasomes, whose properties are to be understood in terms of simple physics.

Lipid Droplets can be regarded as lenses of hydrophobic substance (triacylglycerol, sterol esters) growing up between the two membrane leaflets into micron-large buds, which, possibly, detach from the membrane to form emulsion-like droplets. We address the micromechanics of these organelles to gain understanding of physics behind their formation and evolution.

We analyze the shape and energy of a membrane tubule containing a lipid droplet in dependence of the droplet size and the elastic properties of the tubular membrane and the lipid monolayers covering the droplet surface. We determine the conditions of the droplet detachment from the tubule.

Mini Symposium

Information–theoretical methods for complex systems

Monday, March 27
Lecture Hall, ZIB

Organizers
Sebastian Reich, Carsten Hartmann

Chair
Sebastian Reich

Many natural systems are characterized by their high dimensionality and the presence of many characteristic spatio-temporal scales. A wealth of analytical and computational techniques has been proposed to extract low dimensional models that accurately capture the evolution of certain observables. The systematic use of data in the derivation and validation of the effective models based on information-theoretic tools has been a particularly important development. The mini symposium presents some of the most recent advances in the field.

Speakers

2:30 PM	Manfred Opper
3:00 PM	Michal Branicki
3:30 PM	Valerio Lucarini
4:00 PM	Tim Sullivan

Score matching and nonparametric estimators of drift functions for stochastic differential equations

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Score matching is a technique for estimating probability densities from data. It avoids the complications of computing the normaliser of the density which would be needed, e.g., for maximum likelihood or Bayesian estimators. The method has recently been generalised to a nonparametric setting [3] where it often outperforms more classical techniques such as kernel density estimators.

In this talk I will discuss an application of a generalisation of score matching to the estimation of the drift function $g(\cdot)$ in stochastic differential equations [1] of the form

$$dZ_t = g(Z_t)dt + \sigma(Z_t)dW_t.$$

where $Z \in R^d$ and $D(z) \doteq \sigma(z)\sigma(z)^\top$. The drift $g(z) = r(z) + A(z)\nabla\psi$ is assumed to be composed of known parts $r(\cdot)$ and $A(\cdot)$ but the function $\psi(\cdot)$ has to be estimated from data. I will give applications to second order (Langevin) stochastic differential equations. The method also allows for an estimate of the *relative entropy rate* for path probabilities of two processes [2] and for a sampling based approach to certain optimal control problems.

[1] P. Batz, A. Ruttor, and M. Opper. Variational estimation of the drift for stochastic differential equations from the empirical density. *Journal of Statistical Mechanics: Theory and Experiment*, 330(8):083404, 2016.
[2] M. Opper. An estimator for the relative entropy rate of path measures for stochastic differential equations. *J. Comput. Phys. (C)*, 330:127–133, 2017.
[3] B. K. Sriperumbudur, K. Fukumizu, R. Kumar, A. Gretton, and A. Hyvärinen. Density estimation in infinite dimensional exponential families, 2014.

Multi model density estimators & path-space information theory for stochastic filtering and prediction

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Multi Model Ensemble (MME) predictions are a popular ad-hoc technique for improving predictions of high-dimensional, multi-scale dynamical systems. The heuristic idea behind MME framework is simple: given a collection of models, one considers predictions obtained through the convex superposition of the individual probabilistic forecasts in the hope of mitigating model error. However, it is not obvious if this is a viable strategy and which models should be included in the MME forecast in order to achieve the best predictive performance. I will show that an information-theoretic approach to this problem allows for deriving a sufficient condition for improving dynamical predictions within the MME framework; moreover, this formulation gives rise to systematic and practical guidelines for optimising data assimilation techniques which are based on multi model ensembles. Time permitting, the role and validity of 'fluctuation-dissipation' arguments for improving imperfect predictions of externally perturbed non-autonomous systems will also be addressed.

Response operators for Markov processes in a finite state space: Radius of convergence and link to the response theory for Axiom A systems

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Using straightforward linear algebra we derive response operators describing the impact of small perturbations to finite state Markov processes. The results can be used for studying empirically constructed – e.g., from observations or through coarse graining of model simulations – finite state approximation of statistical mechanical systems. Recent results concerning the convergence of the statistical properties of finite state Markov approximation of the full asymptotic dynamics on the SRB measure in the limit of finer and finer partitions of the phase space are suggestive of some degree of robustness of the obtained results in the case of Axiom A system. Our findings give closed formulas for the linear and nonlinear response theory at all orders of perturbation and provide matrix expressions that can be directly implemented in any coding language, plus providing bounds on the radius of convergence of the perturbative theory. In particular, we relate the convergence of the response theory to the rate of mixing of the unperturbed system. One can use the formulas obtained for finite state Markov processes to recover previous findings obtained on the response of continuous time Axiom A dynamical systems to perturbations, by considering the generator of time evolution for the measure and for the observables. A very basic, low-tech, and computationally cheap analysis of the response of the Lorenz '63 model to perturbations provides rather encouraging results regarding the possibility of using the approximate representation given by finite state Markov processes to compute the system's response [1].

[1] V. Lucarini. Response Operators for Markov Processes in a Finite State Space: Radius of Convergence and Link to the Response Theory for Axiom A Systems. *Journal of Statistical Physics*, 162(2):312–333, 2015.

Probabilistic numerics for differential equations

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Deterministic problems such as matrix inversion, quadrature, optimisation, and the solution of ordinary and partial differential equations are ubiquitous in applied mathematics. With growing demand for uncertainty quantification throughout scientific computing applications, there has been a resurgence of interest in giving probabilistic solutions to such problems, a viewpoint known variously as *Bayesian numerical analysis* [5, 8, 9] or *probabilistic numerics* [6].

In this paradigm, all numerical tasks are interpreted as inference problems, and the role of stochasticity in the algorithm is to replace traditional error bounds as the carriers of epistemic uncertainty about the quality of the solution. Advantages offered by this viewpoint include better propagation of uncertainty through hierarchical systems than simple worst-case error bounds, and appropriate incorporation of numerical truncation and round-off error in inverse problems. In this way, the replicability of deterministic simulations is not confused with their accuracy, a mistake that can yield biased and inappropriately concentrated Bayesian posteriors [4].

This talk will describe recent work on probabilistic numerical solvers for ordinary and partial differential equations, including their theoretical construction, convergence rates, and applications to forward and inverse problems [1–3, 7].
It is joint work with J. Cockayne (Warwick), M. Girolami (Imperial College London), H. C. Lie (FU Berlin), C. Oates (Sydney), and A. M. Stuart (Caltech).

[1] J. Cockayne, C. Oates, T. J. Sullivan, and M. Girolami. Probabilistic meshless methods for partial differential equations and Bayesian inverse problems, 2016. arXiv:1605.07811.
[2] J. Cockayne, C. Oates, T. J. Sullivan, and M. Girolami. Bayesian probabilistic numerical methods, 2017. arXiv:1702.03673.
[3] J. Cockayne, C. Oates, T. J. Sullivan, and M. Girolami. Probabilistic numerical methods for PDE-constrained Bayesian inverse problems, 2017. arXiv:1701.04006.
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[9] J. Skilling. Bayesian solution of ordinary differential equations. In C. R. Smith, G. J. Erickson, and P. O. Neudorfer, editors, *Maximum Entropy and Bayesian Methods*, volume 50 of *Fundamental Theories of Physics*, pages 23–37. Springer, 1992.

Mini Symposium

Multiscale methods for PDEs: Methodology and applications

Monday, March 27
Lecture Hall, Informatik

Organizers
Thomas von Larcher, Reinhold Schneider, Harry Yserentant, Sebastian Wolf

Chair
Reinhold Schneider

Low-rank multilevel approximation methods are an important tool in numerical analysis and in scientific computing. Those methods are particularly suited to attack high-dimensional problems and solutions for nonlinear partial differential equations (PDEs) with high efficiency. In that research area, novel approaches as, e.g., hierarchical tensor product decomposition methods, are promising tools also for application to data that are concerned with cascade-of-scales problems, e.g., in molecular dynamics and in turbulent fluid dynamics. The interdisciplinary character of this session provides mathematical and computational aspects as well as application to data aspects with room for interchanges of ideas and discussions of future work.

Speakers

2:30 PM	Sergey Dolgov
2:55 PM	Vladimir Kazeev
3:20 PM	Thomas von Larcher
3:40 PM	Boris Khoromskij
4:05 PM	Benjamin Stamm

Adaptive spectral time integration of ODEs in the Tensor Train decomposition

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Low-rank tensor product decompositions (the Tensor Train (TT) format [3] in particular) have become a powerful tool for data-sparse approximations of multivariate functions. The singular value decomposition allows to adapt TT ranks to a desired accuracy, and thus optimize the computational costs. On the other hand, an indispensable technique in the standard numerical analysis of PDEs is the adaptive mesh refinement. The next step of research – to combine these two approaches – has emerged recently [1, 2]. I will present a particular instance of this, an adaptation of the polynomial degree in a Chebyshev spectral time discretization and the time interval. A solution of a large linear ODE is sought in the TT format, with the time being one of the variables in the decomposition, discretized on a Chebyshev grid. The resulting linear system is solved via an alternating iteration over TT factors. On top of that, the number of Chebyshev points in time is adapted via an analog of the tau-method. This can be done efficiently from the reduced ODE in the course of the alternating iteration. Moreover, when the number of points exceeds some threshold, the time interval is split, and the system is solved on subintervals. This improves the accuracy by preventing too different snapshots from being approximated in the same TT decomposition. I will demonstrate on numerical examples that this approach can robustly partition long time intervals with a modest overhead.

[1] M. Bachmayr and W. Dahmen. Adaptive low-rank methods: Problems on Sobolev spaces. *SIAM J. Num. Analysis*, 54(2):744–796, 2016.
[2] M. Eigel, M. Pfeffer, and R. Schneider. Adaptive stochastic Galerkin FEM with hierarchical tensor representations. *Numerische Mathematik*, pages 1–39, 2016.
[3] I. V. Oseledets. Tensor-train decomposition. *SIAM J. Sci. Comput.*, 33(5):2295–2317, 2011.

Multilevel structure and tensor approximation: New bounds for analytic and piecewise-analytic functions

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The approximate separation of variables in high-dimensional arrays, or *low-rank tensor approximation*, is mostly seen as an efficient technique for lifting the so-called *curse of dimensionality* in high-dimensional settings. In particular, polynomial approximations are often used in the "physical" and, possibly, parametric spaces to translate a continuous problem into a discrete problem, where the unknowns are collected into a multidimensional array of coefficients, or *tensor*. Polynomial approximations are however known to converge slowly when the solution has low regularity or when the regularity constants of the solution are prohibitively large, which is the case for singular and highly oscillatory solutions. This poses a challenge even in low dimensions, and many discretizations have been developed for such problems, including the adaptive *hp*-FEM and the heterogeneous multiscale method.

As an alternative, an unadapted piecewise-polynomial discretization of low-order based on uniform tensor-product partitions can be used. The accurate approximation of solutions then requires that the discretization be extremely fine, which may inflate the size of the discrete problem algebraically with respect to the desired accuracy. By employing low-rank tensor approximations to resolve the multiscale structure of data and solutions, one may achieve more efficient representation and convergence while retaining such a standard, problem-nonspecific discretization scheme. Recently, the so-called *quantized-tensor-train* (QTT) decomposition has been shown to achieve exponential convergence (with respect to the number of effective degrees of freedom) in certain problems with singular and highly oscillatory solutions. These convergence results build, in particular, upon the tensor-rank bound for the polynomial functions by Grasedyck.

This talk presents refined bounds for the QTT approximation of polynomial and piecewise-analytic functions, based on the subspace interpretation of the QTT decomposition. For a piecewise-analytic function, a characterization of the ranks and accuracy of its QTT approximations in terms of its holomorphy is given and a quasi-optimal adaptive algorithm for QTT approximation with certified accuracy in function norms is proposed.

Tensor product decomposition methods applied to multi-scale data with self-similar characteristics

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Low-rank approximation methods are often suited to attack high-dimensional problems successfully and allow very compact representations of large data sets. Specifically, hierarchical tensor product decomposition methods emerge as an promising approach for application to data that are concerned with cascade-of-scales problems as, e.g., in turbulent fluid dynamics. Here, we focus on two particular objectives, that is representing turbulent data in an appropriate compact form and, secondly and as a long-term goal, finding self-similar vortex structures in multi-scale problems. The question here is whether tensor product methods can support the development of improved understanding of the multi-scale behavior and whether they are an improved starting point in the development of compact storage schemes for solutions of such problems relative to linear ansatz spaces. We discuss the challenges of our approach and present reconstruction capabilities of a tensor product decomposition based modeling approach tested against 3D turbulent channel flow data.

Recent advances in tensor numerical methods for multi-dimensional PDEs

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We discuss how the tensor methods based on the canonical, Tucker, TT and QTT tensor approximation apply to the numerical solution of multi-dimensional PDEs [5, 6], in particular, to calculation of electrostatic potential of lattice-structured systems, to the (post) Hartree-Fock eigenvalue problem for large 3D molecules [1, 3, 4]. We present the recently introduced range-separated (RS) tensor formats [2] which are well suited for rank-structured approximation of many-particle interaction potentials. The particular application is demonstrated on the example of protein modeling via the Poisson-Boltzmann equation. The elliptic equations with highly-oscillating coefficients (homogenization theory) [7] will be also addressed.

[1] P. Benner, S. Dolgov, V. Khoromskaia, and B. N. Khoromskij. Fast iterative solution of the bethe-salpeter eigenvalue problem using low-rank and QTT tensor approximation. *J Comp. Phys.*, (334):221–239, 2017.
[2] P. Benner, V. Khoromskaia, and B. N. Khoromskij. Range-separated tensor formats for numerical modeling of many-particle interaction potentials. *arXiv preprint*, arXiv:1606.09218, 2016.
[3] P. Benner, V. Khoromskaia, and B. N. Khoromskij. A reduced basis approach for calculation of the Bethe-Salpeter excitation energies using low-rank tensor factorizations. *Mol. Physics*, 114(7-8):1148–1161, 2016.
[4] V. Khoromskaia and B. N. Khoromskij. Tensor numerical methods in quantum chemistry: from Hartree-Fock to excitation energies. *Phys. Chem. Chem. Phys.*, 17:31491 – 31509, 2015.
[5] B. Khoromskij. $\mathcal{O}(d \log n)$–Quantics approximation of $N–d$ tensors in high-dimensional numerical modeling. *Constr. Appr.*, 34(2):257–280, 2011.
[6] B. N. Khoromskij. Tensor Numerical Methods for Multidimensional PDEs: Basic Theory and Initial Applications. *ESAIM: Proceedings and Surveys, N. Champagnat, T. Leliévre, A. Nouy, eds*, 48:1–28, January 2015.
[7] B. N. Khoromskij and S. Repin. Grid-based lattice summation of electrostatic potentials by assembled rank-structured tensor approximation. *Russ. J. Numer. Anal. Math. Modelling*, 30(6):329–344, 2015.

An embedded corrector problem for stochastic homogenization

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A very efficient algorithm has recently been introduced in [2] in order to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies in the clever use of a boundary integral formulation of the problem to solve in combination with spherical harmonics. The aim of this talk is to present how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this aim, the definition of new approximate corrector problems and approximate effective coefficients is needed and convergence results in the spirit of [3] are proved for this new formulation [1]. Some numerical test cases will illustrate the behaviour of this method.

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[2] E. Cancès, Y. Maday, and B. Stamm. Domain decomposition for implicit solvation models. *The Journal of Chemical Physics*, 139:054111, 2013.
[3] lain Bourgeat and A. Piatnitski. Approximations of effective coefficients in stochastic homogenization. *Annales de l'institut Henri Poincaré (B) Probabilités et Statistiques*, 40:153–165, 2004.

Mini Symposium

Practical approximations for Monte Carlo simulations of complex systems

Tuesday, March 28
Lecture Hall, ZIB

Organizers
Han Cheng Lie, Tim Sullivan, Carsten Hartmann

Chair
Han Cheng Lie

Many phenomena in the natural sciences and in engineering may be modeled using stochastic dynamical systems. Plain Monte Carlo simulation is the most straightforward computational method for studying the statistics of such systems. However, many of the research projects of the Collaborative Research Centre involve problems caused by rare events, coupled scales, or high-dimensional spaces. The computational cost renders plain Monte Carlo impractical for such problems. This minisymposium focuses on identifying potentially useful tools for and perspectives on Monte Carlo simulation. It emphasises the stochastic nature of the problems, with the purpose of developing better models and more efficient methods.

Speakers

11:30 AM	Ankush Agarwal
12:00 PM	Yannis Pantazis
12:30 PM	Aretha Teckentrup

Rare event simulation related to financial risks: Efficient estimation and sensitivity analysis

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In this paper, we develop the reversible shaking transformation methods on path space to estimate the rare event statistics arising in different financial risk settings which are embedded within a unified framework of isonormal Gaussian process. Namely, we combine splitting methods with both Interacting Particle System (IPS) technique and ergodic transformations using Parallel-One-Path (POP) estimators. We also propose an adaptive version for the POP method and prove its convergence. We demonstrate the application of our methods in various examples which cover usual semi-martingale stochastic models (not necessarily Markovian) driven by Brownian motion and, also, models driven by fractional Brownian motion (non semi-martingale) to address various financial risks. Interestingly, owing to the Gaussian process framework, our methods are also able to efficiently handle the important problem of sensitivities of rare event statistics with respect to the model parameters.

Information-theoretic uncertainty and sensitivity bounds for stochastic dynamics and rare events

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Uncertainty quantification is a primary challenge for reliable modeling and simulation of complex stochastic dynamical systems. Due to their dynamic nature, we need to assess the impact of these uncertainties on the transient and long-time behavior of the stochastic models and derive uncertainty bounds for observables of interest. We present uncertainty and sensitivity bounds for path-space observables of stochastic dynamics in terms of a novel goal-oriented divergence which incorporates both observables and information theory objects such as the relative entropy rate. For sensitivity analysis, the derived bounds rely on the path Fisher Information Matrix. Substituting relative entropy with Renyi entropy, uncertainty and sensitivity bounds for rare events are derived.

Quasi- and multilevel Monte Carlo methods for computing posterior expectations

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The parameters in mathematical models for many physical processes are often impossible to determine fully or accurately, and are hence subject to uncertainty. By modelling the input parameters as stochastic processes, it is possible to quantify the induced uncertainty in the model outputs. Based on available information, a *prior* distribution is assigned to the input parameters. If in addition some dynamic data (or *observations*) related to the model outputs are available, a better representation of the parameters can be obtained by conditioning the prior distribution on these data, leading to the *posterior* distribution in the Bayesian framework.

In most situations, the posterior distribution is intractable in the sense that the normalising constant is unknown and exact sampling is unavailable. Using Bayes' Theorem, we show that posterior expectations of quantities of interest can be written as the ratio of two prior expectations involving the quantity of interest and the likelihood of the observed data. These prior expectations can then be computed using Quasi-Monte Carlo and multilevel Monte Carlo methods.

In this talk, we give a convergence and complexity analysis of the resulting ratio estimators, and demonstrate their effectiveness on a typical model problem in uncertainty quantification.

This is joint work with Rob Scheichl (University of Bath) and Andrew Stuart (Caltech).

Mini Symposium

Deformation accumulation in seismic faults and networks

Tuesday, March 28
Lecture Hall, Informatik

Organizers
Onno Oncken, Matthias Rosenau, Alexander Mielke, Ralf Kornhuber

Chair
Ralf Kornhuber

Earthquake statistics reveal scale invariance over 10 orders of magnitude of the eartquake strength as expressed, e.g., by the famous Gutenberg–Richter power law. However, the scaling properties underlying deformation accumulation in fault networks over longer time scales are virtually unknown. Moreover, because of the incompleteness of the real-world record of earthquakes and deformation accumulation beyond the instrumental and historical time scales (decades to centuries), there is a fundamental lack of insight into the multiscale nature of these processes. In this minisymposium we address mathematical modelling and numerical simulation as well as laboratory scale analogue models and experiments to explore the scaling properties of deformation accumulation in subduction zones and fault networks.

Speakers

11:00 AM	Georg Dresen
11:30 AM	Jean Paul Ampuero
12:00 PM	Alice Gabriel
12:30 PM	Elias Pipping

Faults and shear zones: Relating laboratory tests to geology

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Geological structures and processes often show strong geometric and physical similarities if observed on different scales. Examples range from fractures, faults and shear zones to seismic characteristics such as b-value or seismic source properties. Laboratory tests on small-scale rock samples allow studying aspects of processes that govern earthquake nucleation and rupture propagation, strain localization in shear zones, and high-temperature rheology. However, upscaling of laboratory results to the field scale requires that dominant deformation processes remain the same on vastly different scales, and that potential effects of changing kinematic and thermodynamic boundary conditions may successfully be accounted for by appropriate constitutive equations. A key observational strategy relies on analysis of deformation processes on different scales. In this presentation we will illustrate the approach with two examples from very different geological environments: 1. Scaling of earthquake mechanisms observed in the laboratory, in mines and along major fault zones and 2. High-temperature creep processes governing the deformation in highly localized shear zones in the lower crust and upper mantle. Our results show that constitutive models capturing fundamental physical processes on the laboratory scale may be successfully applied to model deformation on the field scale.

The apparent weakness of active faults

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The strength of fault zones is a key factor controlling plate tectonics and earthquakes. Inferences of stress in the crust from structural and geophysical observations and geodynamic modeling indicate that mature faults are apparently much weaker than expected from classical dry friction. Such inferences actually constrain the large-scale and long-term apparent fault strength. Here, I will examine how the transient nature of earthquake cycles contributes to the apparent weakness of faults, emphasizing the contribution of multi-scale earthquake cycle modeling to this topic.

The weak-fault conundrum arises in part from an implicit assumption that stresses are spatially uniform. In a typical laboratory friction experiment on small samples, slip and stresses are indeed fairly uniform along the sliding surface. Stick-slip on a spring-block model is an appropriate representation of that situation. However, on a long fault embedded in an elastically deforming crust and loaded by deep fault creep, a systematically non-uniform state of stress emerges featuring stress concentrations. This in turn allows earthquakes to nucleate and propagate at low average stresses, leading to low apparent strength. I will describe this mechanism through fracture mechanics theory, earthquake cycle simulations, seismological observations and laboratory experiments.

An integrated view of earthquake source dynamics associated with the 1992 Landers earthquake and the 2004 Sumatra megathrust earthquake

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Capturing the observed complexity of earthquake sources in numerical simulations may require: non-linear fault friction, thermal and fluid effects, heterogeneous fault stress and fault strength initial conditions, fault curvature and roughness, on- and off-fault non-elastic failure. All of these factors have been independently shown to alter earthquake dynamics and thus possibly influence the degree of realism attainable via simulated ground motions.

In this presentation I will show examples of high-resolution earthquake scenarios based on the branched fault network hosting the 1992 Landers earthquake and the 2004 Sumatra megathrust earthquake including splay faults. The dynamic rupture models are performed using SeisSol (`www.seissol.org`), a software package based on an ADER-Discontinuous Galerkin scheme for solving the spontaneous dynamic earthquake rupture earthquake rupture with high accuracy in both space and time. SeisSol utilises unstructured tetrahedral meshes, thereby allowing for a realistic representation of the non-planar fault geometry, subsurface structure and bathymetry. The simulations I will present combine a multitude of representations of source complexity at the necessary spatio-temporal resolution. The latter point is achieved by using large-scale HPC systems, and more importantly, due to the excellent parallel scalability of the implementations within SeisSol.

The high-resolution dynamic rupture models allow an analysis of the dominant factors impacting earthquake source physics and ground motions. Across all simulations, we find that fault geometry concurrently with the regional background stress state provide a first order influence on source dynamics and the emanated seismic wave field. Off-fault Drucker-Prager plastic yielding increases in areas of higher structural complexity and impacts the spatio-temporal rupture patterns as well as macroscopic earthquake source characteristics. I will conclude with an outlook examining the coupling of scenario-based dynamic rupture simulations to geodynamic seismic cycle models models in an effort to provide a self consistent initial condition for the state of stress, strength and fault geometry required by the dynamic rupture problem.

Rate-and-state friction: From analysis to simulation

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We introduce a variational formulation for the sliding motion of viscoelastic bodies against rigid media with rate-and-state friction – a type of motion that plays an important role in the modelling of earthquake rupture. We discuss existence of solutions [1] and present a mathematically consistent numerical algorithm featuring adaptive time stepping as well as a novel algebraic solution algorithm involving fixed-point iteration and multigrid. A laboratory scale subduction zone serves as a testbed for our algorithm, allowing us to show its robustness and carry out a comparison with experimental results [2]. Extensions to the case of sliding against deformable media are also discussed.

[1] E. Pipping. Existence of long-time solutions to dynamic problems of viscoelasticity with rate-and-state friction. Preprint, SFB 1114, 2017.
[2] E. Pipping, R. Kornhuber, M. Rosenau, and O. Oncken. On the efficient and reliable numerical solution of rate-and-state friction problems. *Geophysical Journal International*, 204(3), 2016.

Mini Symposium

Stochastic parametrizations for convective processes

Tuesday, March 28
Lecture Hall, ZIB

Organizers
Uwe Ulbrich, Henning Rust, Christian Franzke, Rupert Klein

Chair
Christian Franzke

Convective processes play an important role in atmospheric dynamics. However, even state-of the art global circulation models still exhibit systematic biases in representing these processes since they act on scales comparable to or smaller than the grid scale. Alternatively to capturing their effect by parametric functions, stochastic models are now increasingly used to systematically represent the highly variable nature of these processes. Our Mini-Symposium will discuss a wide range of stochastic approaches.

Speakers

2:30 PM	Boualem Khouider
2:55 PM	Robert Plant
3:20 PM	Axel Seifert
3:45 PM	Glen Shutts
4:10 PM	Alexander Kuhn

Stochastic multi-cloud models for the parameterization of organized tropical convection

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Tropical convection is organized on a hierarchy of scales that interact with each other and with the large-scale flow. Efforts to adequately represent these convective systems in a global climate model (GCM) has led the scientific community to think beyond conventional convective parameterization schemes. Super-paramaterized GCMs (SP-GCM) and global cloud resolving models (GCRM) are such promising approaches. While the high computational cost inhibited the widespread use of SP-GCMs and GCRMs operationally, they highlighted the importance of the representation of sub-grid scale variability collectively while realizing the individual behaviour of the convective elements. I will discuss a new perspective of stochastic multicloud models (SMCM), based on Markov lattice models, to represent the sub-grid scale organization of convection and its two-way interaction with large-scale tropical waves. Building up from simple models for convectively coupled waves to their implementation in GCMs, I will demonstrate the importance of three key cloud types (congestus, deep and stratiform) as a building block for organized convection. Results showing significant improvements in the capability and superiority of the SMCM to capture synoptic and intra-seasonal variability associated with tropical convection, in GCMs, including convectively coupled equatorial waves, the Madden-Julian oscillation and monsoon intraseasonal oscillations, will be presented.

Stochastic aspects of convection-permitting models

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Atmospheric convective processes are incorporated within climate modelling and global numerical weather prediction by means of a parameterization, which aims to represent the effects of the convective motions on the larger, resolved-scale flow. There is ever-increasing evidence that it can be beneficial for the parameterization to be stochastic, reflecting the fact that a wide range of possible realizations of the unresolved processes may be entirely consistent with the resolved-scale model state.

Convective processes may also be simulated directly, without the need for parameterization, if the model resolution is fine enough and if results are wanted over a limited length or timescale. Direct simulation has relatively recently become common practice for 1–2 day national-scale weather forecasting, as well as for research studies of convection. This talk will discuss the possible inclusion of stochastic effects for such fine-resolution convection-permitting simulations. Why might stochastic effects continue to be important for such simulations? What is the physical origin of the uncertainty to be represented? How might the uncertainties be represented in simple and justifiable ways? Do the uncertainties actually need to be captured within simulations themselves, or would a simple statistical post-processing be sufficient?

We do not have good answers to such questions yet, but experimentation is now well under way in various groups and our experiences with parameterized–convection models might provide us with some useful clues. Simple pragmatic methods applied at large scales have been trialled. Some of the arguments developed through consideration of convection in larger-scale models might reasonably be extended to the consideration of uncertainties in parameterizing turbulence. Unfortunately, some difficulties familiar from larger-scale modelling seem likely to remain relevant too. The key questions also overlap strongly with emerging issues around appropriate methods for the interpretation and evaluation of model results at convective scales.

A stochastic model of shallow convection in the atmosphere

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Shallow cumulus convection plays an important role in the atmosphere and is a major uncertainty in climate and numerical weather prediction (NWP) models. In all climate and NWP models shallow convection acts on scales smaller than the numerical mesh size and, hence, needs to be modeled by sub-grid parameterizations. In NWP models with grid spacings of order 1 km the deeper modes of convection are at least partly resolved, but shallow convection remains a sub-grid process. Especially on such scales the shallow convective clouds act as a random stochastic process and classic Reynolds-averaged models are insufficient to parameterize the effect of sub-grid clouds. Using large-eddy simulations that are able to resolve all relevant convective scales the properties of the shallow convective cloud field can be investigated and theoretical models can be tested rigorously. A stochastic model based on a compound Poisson process is introduced to describe the variability of the sub-grid cloud processes. The assumed probability distribution depends on certain physical properties of the cloud field like the cloud size distribution and the cloud lifetime. It is shown that such a stochastic process can replicate the statistics of the large-eddy simulations for the most important quantities like cloud fraction and cloud mass flux. This stochastic process can then be coupled with a classic mass flux parameterization of shallow convective clouds. It is shown that the stochastic parameterization improves certain aspects of the overall model behavior, but a physically consistent description of cloud processes across a wide range of scales remains challenging.

Representing uncertainty associated with mesoscale convective systems

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The triggering and growth of individual cumulus clouds is known to be highly sensitive to details of the boundary layer (and underlying surface) together with the temperature, wind and humidity of the environment above. This potential lack of predictability associated with random,turbulent fluctuations in boundary layer state is mitigated somewhat by the fact that topography, land type, lakes and coastlines exert strong control over where convection is likely to occur. For instance, wind convergence associated with sea breeze fronts can force convective clouds, thereby inheriting some of the predictability of the sea breeze phenomenon itself.

Convective systems are manifest on many atmospheric space and time scales e.g. from kilometre-scale cumulus clouds to organized Mesoscale Convective Systems (MCSs) stretching over hundreds of kilometres. A characteristic feature of convection is that their individual updraughts tend to be on the kilometre scale or smaller – even for MCSs. A consequence of this fact is that, in spite of their large size relative to typical gridlengths of global weather forecast models (10 to 30 km), MCSs are poorly represented. Added to this is the sensitivity of even these large systems to flow details in the boundary layer (e.g., the spreading of cold pools from previous convective events) and mesoscale forcing of vertical motion associated with upper tropospheric flow features, e.g., jet streaks. Unlike a field of fair-weather cumulus clouds over land (or convective polar airstreams moving equatorward over warm waters), MCSs are large enough and of sufficient duration to engage the Earth's rotation and the vertical redistribution of mass they bring about creates potential vorticity features and attendant cyclonic and anticyclonic circulations. These are of sufficient scale to influence the evolution of growing baroclinic waves within which they develop. The aforementioned sequence of events therefore provides a mechanism for upscaling forecast errors for highly convectively-unstable regions outside of the tropics.

In the context of ensemble forecasts, a technique ([1]) for representing this random forecast error due to MCSs will be presented. It works by introducing a vorticity and divergence forcing function centred on all grid columns with parametrized convection. The forcing is driven through the parametrized deep convective mass flux as a first-order auto-regressive process and smoothed horizontally. Results from its use in the ECMWF ensemble prediction system, and from its offline application to an explicit simulation of an MCS, will be presented.

[1] G. Shutts. A stochastic convective backscatter scheme for use in ensemble prediction systems. *Q.J.R. Meteorol. Soc.*, 141:2602–2616, 2015.

Object-based visualization and evaluation of cloud-resolving simulations

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Recent advances in high-resolution, cloud resolving simulation models pose several challenges towards respective analysis methodologies. To enable efficient comparison and validation of such models efficient, scalable, and informative diagnostic procedures are mandatory. In this talk, an object-based evaluation scheme based on the notion of scalar field topology will be presented. The presentation will cover the application of topological clustering procedures for object identification, tracking, and the retrieval of object-based statistics. The proposed methodology is shown to enable an advanced in-depth evaluation and visualization of high cloud-resolving models. Using a newly developed large-scale high-resolution model (i.e., HD(CP)^2 ICON) It will be demonstrated that the presented procedures are applicable to assess the model performance compared to measurements (e.g., radar, satellite) and standard operational models (COSMO) at different domains and spatial scales.

Mini Symposium

Coarse graining in molecular systems

Tuesday, March 28
Lecture Hall, Informatik

Organizers
Stefan Klus, Christof Schütte, Ralf Kornhuber

Chair
Christof Schütte

The ever-increasing complexity of molecular systems renders an efficient numerical analysis virtually impossible. The basic idea behind coarse graining is to replace the high-dimensional all-atom description of such systems by a reduced representation that preserves the properties of interest with a sufficient accuracy. The goal of the minisymposium is to present and discuss novel approaches for the systematic derivation of coarse grained models, their numerical realization with a focus on data-driven methods, and their validation based on both mathematical insight and real-life experiments.

Speakers

2:30 PM	Wei Zhang
3:00 PM	Cecilia Clementi
3:30 PM	Stefan Klus
4:00 PM	Peter Koltai

Model reduction of diffusion process along reaction coordinate and related topics

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Projecting a high-dimensional stochastic dynamics on the reaction coordinate space has attracted considerable attentions in the literature. In this talk, I will discuss the model reduction of a diffusion process along certain given reaction coordinate. The main focus will be the properties which are inherited from the original dynamics, as well as error estimates of the timescales and reaction rates of the projected dynamics comparing to those of the full dynamics. Several algorithmic issues will be discussed as well. This talk is mainly based on the work [1].

[1] W. Zhang, C. Hartmann, and C. Schütte. Effective dynamics along given reaction coordinates, and reaction rate theory. *Faraday Discuss.*, 195:365–394, 2016.

TITLE TBA

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[no abstract]

Data-driven transfer operator approximation

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In this talk, we will present tensor-based reformulations of data-driven methods such as Dynamic Mode Decomposition (DMD) and Extended Dynamic Mode Decomposition (EDMD) for the analysis of complex dynamical systems. Due to the curse of dimensionality, analyzing high-dimensional systems is often infeasible using conventional methods since the amount of memory required to compute and store modes and eigenfunctions grows exponentially with the size of the system. This can be mitigated by exploiting low-rank tensor approximation approaches. We will show how tensor-based methods can be used to approximate the eigenfunctions of transfer operators. The results are illustrated with the aid of simple fluid dynamics and molecular dynamics examples.

Markov state models for nonequilibrium molecular dynamics

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[no abstract]

Mini Symposium

Open systems

Wednesday, March 29
Lecture Hall, ZIB

Organizers
Rupert Klein, Luigi Delle Site, Christof Schütte, Carsten Hartmann

Chair
Carsten Hartmann

Physical modelling, mathematical formalisation and numerical simulation of open systems is becoming more and more important for a broad field of applications, ranging from quantum computers to biological systems out of equilibrium. A common theme is that the applications require a precise and systematic modelling of the interaction of the system of interest with its environment, while being subject to computational constraints that limit the achievable level of detail in these models.

The talks in this minisymposium offer a look at the most recent advances in the field and include state-of-the art methods for modelling, simulating and analysing open systems.

Speakers

11:00 AM	Patrick Ilg
11:30 AM	Michela Ottobre
12:00 PM	Matej Praprotnik
12:30 PM	Jens Eisert

Internal structure and dynamics of complex fluid interfaces

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The interface region through which open systems exchange energy and matter shows many interesting properties in case of complex fluids such as colloids, liquid crystals, polymers, etc. We here show some examples of nanoparticle-stabilized interfaces [2, 4] as well as assemblies of block co-polymers at interfaces. Furthermore, we present a systematic coarse-graining study for deriving the interface rheology of liquid-crystalline systems starting from microscopic model systems [3]. As a proof of principle, we consider the idealized situation of a perfectly planar interface and hard ellipsoidal particles. For this case, we derive the effective free energy from a large-deviation rate function, the deterministic drift from the Poisson bracket approach, and effective friction forces by evaluating the corresponding expression from Mori–Zwanzig projection operator approach [1]. Finally, some remarks towards modeling the transport problem through such interfaces are offered.

[1] P. Ilg, V. G. Mavrantzas, and H. C. Öttinger. Multiscale modeling and coarse graining of polymer dynamics: Simulations guided by statistical beyond-equilibrium thermodynamics. In P. D. Gujrati and A. L. Leonov, editors, *Modeling and Simulations in Polymers*. Wiley-Interscience, 2010.
[2] L. Isa, E. Amstad, K. Schwenke, E. D. Gado, P. Ilg, M. Kröger, and E. Reimhult. Adsorption of core-shell nanoparticles at liquid-liquid interfaces. *Soft Matter*, 7:7663–7675, 2011.
[3] A. Luo, L. Sagis, H. Öttinger, C. D. Michele, and P. Ilg. Modelling the rheology of anisotropic particles adsorbed on a two-dimensional fluid interface. *Soft Matter*, 11:4383–4395, 2015.
[4] Z. A. Zell, L. Isa, P. Ilg, L. G. Leal, and T. M. Squires. Adsorption energies of poly(ethylene oxide)-based surfactants and nanoparticles on an air-water surface. *Langmuir*, 30:110–119, 2013.

Sampling with non-reversible dynamics

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In recent years the observation that "irreversible processes converge to equilibrium faster than their reversible counterparts" has sparked a significant amount of research to exploit irreversibility within simulation and sampling schemes. It is now understood how to design irreversible continuous time dynamics with prescribed invariant measure. However, for sampling/simulation purposes, such dynamics still need to undergo discretization and, as it is well known, naive discretizations can completely destroy all the good properties of the continuous-time process.

In this talk we will (i) give an overview of the different sampling and simulation approaches taken so far in this context (ii) present some of the available non-reversible Markov Chain Monte Carlo algorithms (iii) make further considerations on how (not) to use irreversibility within Markov Chain Monte Carlo algorithms.

Work in collaboration with N. Pillai (Harvard), A. Stuart (Caltech), F. Pinski (Cincinnati) and K. Spiliopoulos (Boston).

Open boundary molecular dynamics

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Open molecular systems exchange mass, momentum, and energy with their surroundings. In this talk, I will present our Open Boundary Molecular Dynamics (OBMD) method that opens up the boundaries of a molecular system and allows for equilibrium MD simulations in the grand-canonical ensemble as well as nonequilibrium fluid flow simulations [1]. The flow is introduced via an external boundary condition while the equations of motion for the bulk remain unaltered. To illustrate the robustness of OBMD, I will present simulation results of star-polymer melts at equilibrium and in sheared flow [2].

[1] R. Delgado-Buscalioni, J. Sablić, and M. Praprotnik. Open boundary molecular dynamics. *Eur. Phys. J. Special Topics*, 224:2331–2349, 2015.
[2] J. Sablić, M. Praprotnik, and R. Delgado-Buscalioni. Open boundary molecular dynamics of sheared star-polymer melts. *Soft Matter*, 12:2416–2439, 2016.

Theory and simulation of open quantum systems

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All physical system are to some extent open, and quantum systems are no exception to this rule. Open system dynamics is usually seen as a foe, leading to unwanted decoherence and dissipation. It has recently turned out, however, that in important instances, open system dynamics can be put to a good use. In this talk, we will discuss such open quantum systems. At the heart of the talk will be new methods [3] based on tensor networks [1, 2] – generalizing ideas of tensor trains – for their efficient numerical study, linking the study of open quantum systems to other related endeavors in the CRC 1114.

[1] J. Eisert. Entanglement and tensor network states. *Modeling and Simulation*, 3(520), 2013.
[2] J. Eisert, M. Cramer, and M. B. Plenio. Area laws for the entanglement entropy. *Rev. Mod. Phys.*, 82(277), 2010.
[3] A. H. Werner, D. Jaschke, P. Silvi, T. Calarco, J. Eisert, and S. Montangero. A positive tensor network approach for simulating open quantum many-body systems. *Phys. Rev. Lett.*, 116(237201), 2016.

Mini Symposium

Molecular kinetics and kinetic models from MD simulations

Wednesday, March 29
Lecture Hall, Informatik

Organizers
Roland Netz, Robert Schulz, Julian Kappler, Jan Daldrop, Frank Noe, Robert Patterson

Chair
Douwe Bonthuis

Gaining molecular insights into nanoscale kinetics from Molecular Dynamics (MD) simulations is challenging due to the large number of degrees of freedom involved and the limited computational power. This mini-symposium addresses applied and conceptual questions: An important issue of all-atom MD simulations is that physically relevant processes typically happen on time scales much larger than simulation time. Novel techniques to overcome this sampling problem, based on applying external bias potentials to collective variables, will be discussed. A separate issue concerns the meaningful analysis of simulation trajectories and the connection to experimental data. As an example, the translational and orientational dynamics of hydration water close to a biomolecular surface will be discussed.

Speakers

11:00 AM	Matthias Heyden
11:40 AM	Omar Valsson
12:20 PM	Nuria Plattner

Connecting local solvent dynamics to thermodynamic properties

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Rate constants for self-diffusion and orientational relaxation of solvent molecules in heterogeneous chemical environments provide partial information on the local free energy surface, in particular kinetic barriers involved in the corresponding dynamic processes. Experimental techniques such as Overhauser dynamic nuclear polarization [2] or nuclear magnetic relaxation [3] are sensitive to such local dynamical processes in the environment of either artificial labels or near specific functional groups. In site-resolved measurements of solvated biomolecules, i.e. proteins, such experiments can provide sophisticated maps that characterize the local hydration water dynamics on the entire biomolecular surface.

Here, we use molecular dynamics simulations in order to investigate the experimental maps of local hydration water dynamics within the employed simulation models. We combine this analysis with a spatially resolved thermodynamic decomposition, which allows the investigation of local contributions to solvation free energies. The specific approach enables us to separate energetic and entropic consequences of interactions between water and the biomolecular solute as well as of changes in the solvent structure.

We then investigate the amount of local thermodynamic information that can be obtained from simulated or experimental observations of local hydration water dynamics, inspired, for example, by a previously derived universal scaling law [1] that relates the excess entropy and self-diffusion rates in atomic fluids.

In particular, we show that local translation and reorientation dynamics conveys information on local hydration water entropies, while at the same time more detailed conclusions on binding free energies are impeded by compensating variations in the local hydration water energy and entropy.

[1] M. Dzugutov. A universal scaling law for atomic diffusion in condensed matter. *Nature*, 381:137–139, 1996.
[2] O. Fisette, C. Päslack, R. Barnes, J. M. Isas, R. Langen, M. Heyden, S. Han, and L. Schäfer. Hydration dynamics of a peripheral membrane protein. *J. Am. Chem. Soc.*, 138:11526–11535, 2016.
[3] N. V. Nucci, M. S. Pometun, and A. J. Wand. Mapping the hydration dynamics of ubiquitin. *J. Am. Chem. Soc.*, 133:12326–12329, 2011.

Enhancing important fluctuations and exploring free landscapes with variationally enhanced sampling

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The usefulness of atomistic simulations is generally hampered by the presence of several metastable states separated by high barriers leading to kinetic bottlenecks. Transitions between metastable states are thus rare events that occur on much longer time scales than one can simulate in practice. Numerous enhanced sampling methods have been suggested to alleviate this time scale problem, including methods based on identifying a few crucial order parameters or collective variables and enhancing their fluctuations through the introduction of an external biasing potential [5].

Here will we discuss Variationally Enhanced Sampling [4], a new generally applicable enhanced sampling method which is based on a rigorous variational principle [4]. In this approach an external bias potential that acts in the space spanned by the collective variables is constructed by minimizing a convex functional. The underlying free energy landscape as a function of the selected collective variables can be obtained directly from the bias that minimizes this functional. We present numerous examples which show the flexibility, practicality, and usefulness of the method. We will furthermore discuss how the variational property of the method can be used to extend the method in novel and innovative ways, including for example: to obtain kinetic information from atomistic simulation [1]; to sample high dimensional free energy surfaces [3]; and to accelerate nucleation events by employing a physical model from classical nucleation theory [2].

[1] J. McCarty, O. Valsson, P. Tiwary, and M. Parrinello. Variationally optimized free-energy flooding for rate calculation. *Physical Review Letters*, 115:070601, 2015.
[2] P. M. Piaggi, O. Valsson, and M. Parrinello. A variational approach to nucleation simulation. *Faraday Discuss.*, 195:557–568, 2016.
[3] P. Shaffer, O. Valsson, and M. Parrinello. Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin. *Proceedings of the National Academy of Sciences*, 113:1150–1155, 2016.
[4] O. Valsson and M. Parrinello. Variational approach to enhanced sampling and free energy calculations. *Physical Review Letters*, 113:090601, 2014.
[5] O. Valsson, P. Tiwary, and M. Parrinello. Enhancing important fluctuations: Rare events and metadynamics from a conceptual viewpoint. *Annual Review of Physical Chemistry*, 67:159–184, 2016.

Kinetics of protein-ligand binding and protein-protein interactions revealed in atomic detail using Markov state modeling

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Markov state modeling in combination with high-throughput molecular dynamics (MD) simulations is a tool which allows to overcome the parallelization limit and resolve the kinetics of complex systems. [1] This method has been used successfully to build models of protein-ligand interactions for the serine protease Trypsin and its competitive inhibitor Benzamidine [4], as well as to describe detailed interactions of the ribonuclease Barnase and its natural inhibitor Barstar [3]. It is demonstrated how Markov state modeling can be used to summarize the complex kinetics of protein-ligand binding and protein-protein interactions in multi-state models which can then be used to predict functionally relevant observables of these system over long timescales. For Trypsin/Benzamidine the interplay between different protein conformations and ligand binding has been assessed, providing direct evidence of conformational plasticity in Trypsin-like serine proteases. [4] For Barnase/Barstar protein-protein association and dissociation has been resolved in full atomic detail using a hidden Markov model [2]. The proteins initially associate into a structurally diverse set of non-native encounter states. This ensemble eventually funnels into an intermediate transition state in which Barnase and Barstar are flexibly associated by a few key amino acids. Reaching the final bound configuration requires tens of microseconds after the initial encounter. The bound state fluctuates on the microseconds timescale, between a more stable substate and a less tightly bound and flexible substate. The complex remains stable for minutes, and exhibits multiple geminate rebinding events through non-native intermediates prior to dissociating with the expected experimental kinetics. [3]

[1] G. R. Bowman, V. S. Pande, and F. Noé, editors. *An Introduction to Markov State Models and Their Application to Long Timescale Molecular Simulation.*, volume 797 of *Advances in Experimental Medicine and Biology*. Springer, Heidelberg, 2014.
[2] F. Noé, H. Wu, J.-H. Prinz, and N. Plattner. Projected and hidden Markov models for calculating kinetics and metastable states of complex molecules. *J. Chem. Phys.*, 139:184114, 2013.
[3] N. Plattner, G. D. Fabritiis, S. Doerr, and F. Noé. Protein-protein association and binding mechanism resolved in atomic detail. *submitted*.
[4] N. Plattner and F. Noé. Protein conformational plasticity and complex ligand binding kinetics explored by atomistic simulations and Markov models. *Nature Commun.*, 6:7653, 2015.

Mini Symposium

Stochastic modeling approaches for turbulent flows

Wednesday, March 29
Lecture Hall, ZIB

Organizers
Thomas von Larcher, Nikki Vercauteren, Rupert Klein

Chair
Thomas von Larcher

Turbulent flows are characterised by complex spatio-temporal dynamics involving multifaceted cascade-of-scales problems. The efficient modeling particularly of sub-grid scale turbulence requires understanding of the physics and statistics of scale interactions and has been a subject of intensive research over the past decades. Novel approaches as, e.g., stochastic/statistical methods and data-driven models, have been recently developed to analyse and represent scale interactions in hydrodynamic turbulence. The session provides discussions about recent developments and gives room for an exchange of ideas for future work.

Speakers

2:30 PM	Davide Faranda
2:55 PM	Nikki Vercauteren
3:15 PM	Jeroen Wouters
3:40 PM	Christian Franzke
4:05 PM	Fenwick Cooper

Stochastic chaos in a turbulent von Karman flow

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SPEC, CEA, CNRS,
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We discuss the existence of a low-dimensional attractor in time-series issued from a laboratory model fluid in highly turbulent conditions. Our reconstruction is based on the combination of tools from dynamical systems theory and on ideas borrowed from the field of stochastic processes. The results demonstrate the possibility the behavior of a turbulent flow with a dynamical system with fluctuating control parameter. Such fluctuations represent, via a noise term, the influence of the small scales on the dynamics.

In our experiment, we generate turbulence in a vertical cylinder go length $H = 180$ mm and radius $R = 100$ mm filled with water, and stirred by two coaxial, contra-rotating impellers with rotating frequency f_1 and f_2 and torque C_1 and C_2. Due to the symmetry of our experimental set-up, we choose $\gamma = (C_1 - C_2)/(C_1 + C_2)$ as the control parameter. The θ parameter is a global quantity, tracing deviations from the top-bottom symmetry in the flow. by embedding the partial maxima θ_m in a three dimensional space, we can reconstruct the associated turbulent attractor as a function of the average forcing γ imposed. When $\gamma = 0$ the top and the bottom impeller are exchangeable. In absence of any symmetry breaking mechanism, we expect the flow to react such that $\theta = (f_1 - f_2)/(f_1 + f_2)$ is also zero. Therefore the embedding of θ returns just a noisy fixed point. For increasing $|\gamma|$, first an unstable limit cycle appears, then the cycle stabilizes and and bifurcates again in another limit cycle [1]. The full attractors consists of three limit cycles (arrows) and two quasi-stationary states s_1 and s_2.

We further show that the experimental attractor can be modeled by stochastic Duffing equations, that match the quantitative properties of the experimental flow, namely the number of quasi-stationary states and transition rates among them, the effective dimensions, and the continuity of the first Lyapunov exponents. Such properties can neither be recovered using deterministic models nor using stochastic differential equations based on effective potentials obtained by inverting the probability distributions of the experimental global observables. Our findings open the way to low dimensional modeling of systems featuring a large number of degrees of freedom and multiple quasi-stationary states.

[1] D. Faranda, Y. Sato, B. Saint-Michel, C. Wiertel, V. Padilla, B. Dubrulle, and F. Daviaud. Stochastic chaos in a turbulent swirling flow. *arXiv preprint arXiv:1607.08409*, 2016.

Flow regimes and scale interactions in the stably stratified atmospheric boundary layer

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Boundary-layer turbulence in stably stratified weak-wind conditions is typically intermittent and generated partly by shear associated with propagating non-turbulent motions on the so-called submesoscales (corresponding roughly to scales smaller than 2km). If they are sufficiently strong, local bursts of turbulent mixing due to submesoscale propagating motions can (but do not necessarily) drive transitions from strong to weak stable stratification. Little is known about the specific physical mechanisms that drive intermittent turbulence and transitions between strong stable stratification, where the turbulence is nearly suppressed, and weak stable stratification, where turbulence is weak but continuous. In this talk I will present data-driven methods for identifying different regimes of stably stratified atmospheric flows based on the interactions between submesoscale motions and turbulence. I will discuss how such data-driven flow classifications could help deriving stochastic closures for stable boundary layer flows, which are so far poorly represented in weather forecast models.

Beyond the limit of infinite time-scale separation: Edgeworth approximations and homogenisation

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Homogenization has been widely used in stochastic model reduction of slow-fast systems, including geophysical and climate systems. The theory relies on an infinite time scale separation. In this talk we present results for the realistic case of finite time scale separation. In particular, we employ Edgeworth expansions as finite size corrections to the central limit theorem and show improved performance of the reduced stochastic models in numerical simulations. This is joint work with Georg Gottwald.

Energy conserving stochastic models of the atmosphere

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Stochastic methods are more and more widely used in numerical weather and climate prediction models in order to represent the impact of unresolved scales and processes. It has been shown that stochastic terms in the equations lead to considerable improvements in forecast skill and bias reduction [1, 2, 6]. However, most of these stochastic approaches are ad hoc. Whether these schemes conserve quantities like energy and momentum is unclear. One systematic approach, the stochastic mode reduction [4, 5, 8, 9], is nonlinearly stable but its energy consistency has not been shown so far.

Here we will present a systematic way of deriving energy conserving stochastic models of the 2-layer Quasi-Geostrophic equations and the compressible non-hydrostatic equations. This is based on the projection operator approach developed by [3]. The energy conservation constraint leads to multiplicative noise and nonlinear damping terms. I will also discuss the effects of memory in stochastic modelling [7]. Stochastic modelling is based on the implicit assumption of a time scale separation. However, there is no evidence for a time scale separation in the atmosphere. This lack of time scale separation leads to the emergence of memory effects. Such effects are ignored in most current stochastic parameterization schemes.

This work is supported by the German Research Foundation (DFG) through the Collaborative Research Center SFB/TRR 181 'Energy Transfers in Atmosphere and Ocean' at the University of Hamburg.

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[2] J. Berner, G. Shutts, M. Leutbecher, and T. Palmer. A spectral stochastic kinetic energy backscatter scheme and its impact on flow-dependent predictability in the ecmwf ensemble prediction system. *J. Atmos. Sci.*, 66:603–626, 2009.
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Optimisation of an idealised primitive equation ocean model using stochastic parameterization

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Using a simple parameterization, an idealised low resolution (biharmonic viscosity coefficient of 5×10^{12} $m^4 s^{-1}$, 128×128 grid) primitive equation baroclinic ocean gyre model is optimised to have a much more accurate climatological mean, variance and response to forcing, in all model variables, with respect to a high resolution (biharmonic viscosity coefficient of 8×10^{10} $m^4 s^{-1}$, 512×512 grid) equivalent. For example, the change in the climatological mean due to a small change in the boundary conditions is more accurate in the model with parameterization. Both the low resolution and high resolution models are strongly chaotic.

This work [1] extends earlier work that considered a shallow water barotropic gyre [2]. The parameterization consists of a constant forcing, applied to the velocity and temperature equations at each grid point, which is optimised to obtain a model with an accurate climatological mean, and a linear stochastic forcing, that is optimised to also obtain an accurate climatological variance and 5 day lag auto-covariance. A linear relaxation (nudging) is not used.

[1] F. C. Cooper. Optimisation of an idealised primitive equation ocean model using stochastic parameterization. *Ocean Modelling*, 2016.
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Mini Symposium

Multi-scale reaction kinetics

Wednesday, March 29
Lecture Hall, Informatik

Organizers
Mohsen Sadeghi, Frank Noé, Christoph Fröhner, Luigi Sbailò, Moritz Hoffmann

Chair
Mohsen Sadeghi

Multi-scale reaction kinetics methods are used to study complex reactive systems. Examples are chemical signaling in living cells, ligand binding and catalytic reactions. These processes range in scales from nanoseconds to seconds in time, and from few nanometers to several micrometers in space. It is usually challenging to efficiently simulate reactive systems over different scales. However, several methods have been developed to successfully deal with multi-scale systems, these methods mainly use two different approaches. In concentration-based approaches the volume is divided into subvolumes of constant particle density, whereas particle-based approaches explicitly account for every particle in the system. This minisymposium is aimed at presenting a selection of these methods.

Speakers

2:30 PM	Pieter Rein ten Wolde
3:10 PM	Matthias Weiss
3:50 PM	Stefanie Winkelmann

Combining molecular dynamics with mesoscopic Green's function reaction dynamics simulations

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In many reaction-diffusion processes, ranging from biochemical networks, catalysis, to complex selfassembly, the spatial distribution of the reactants and the stochastic character of their interactions are crucial for the macroscopic behavior. The recently developed mesoscopic Green's Function Reaction Dynamics (GFRD) method enables efficient simulation at the particle level provided the microscopic dynamics can be integrated out. Yet, many processes exhibit non-trivial microscopic dynamics that can qualitatively change the macroscopic behavior, calling for an atomistic, microscopic description. I present a novel approach that combines GFRD for simulating the system at the mesoscopic scale where particles are far apart, with a microscopic technique such as Langevin dynamics or Molecular Dynamics (MD), for simulating the system at the microscopic scale where reactants are in close proximity. The new multi-scale scheme, called MD-GFRD, is generic and can be used to efficiently simulate reaction-diffusion systems at the particle level.

Move before reacting – multi-scale motion of molecules in biological/bio-mimetic fluids

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[no abstract]

The spatiotemporal chemical master equation

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The spatiotemporal chemical master equation (ST-CME) is a model for stochastic reaction-diffusion kinetics which exhibit properties of metastability. With the space of motion being coarse-grained into metastable subvolumes, diffusion is approximated by a discrete jump process between the subvolumes and reactions can take place between reactive species located in the same subvolume. Treating the diffusive jumps as unimolecular reactions, the ST-CME is formally a chemical master equation, such that the associated numerical simulation methods (such as Gillespie's algorithm) can directly be applied. Formally, the ST-CME emerges from a Galerkin projection of the more detailed particle-based dynamics. We present the ST-CME as an intuitive coarse-graining approach and reveal both its theoretical background as well as suitable applications.

[1] S. Winkelmann and C. Schütte. The spatiotemporal master equation: Approximation of reaction-diffusion dynamics via Markov state modeling. *The Journal of Chemical Physics*, 145(21):214107, 2016.

Poster Session

ZIB Foyer

With fingerfood and drinks provided, you will have the opportunity to get to know other researchers, network, and have a close look at the posters displayed.

Coupling a multiscale stochastic precipitation model to large scale atmospheric flow dynamics (A01)

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Precipitation is one of the atmospheric processes with the highest spatio-temporal variability. Additionally, it exhibits very different characteristics on multiple scales. Poisson cluster processes are frequently used as stochastic precipitation models. Besides using them to simulate time series or spatio-temporal precipitation fields for, e.g., hydrological applications, they share some characteristics with stochastic parametrizations for convection. Here, we investigate a particular Poisson cluster model with respect to its ability to reproduce multi-time-scale characteristics of observations.

Furthermore precipitation is associated with the release of latent heat within the atmosphere, a diabatic process. Diabatic processes and non-stationarity can be identified by means of the Dynamic State Index (DSI). This index indicates local deviations of the atmospheric flow field from a stationary, inviscid and adiabatic solution of the primitive equations of fluid mechanics. It can be applied to diagnose and even prognose atmospheric flow phenomena on different scales. On the convective scale, it is highly correlated with precipitation.

We seek a functional relationship between the parameters of the Poisson cluster precipitation model and variables from the deterministic root model. These relations can be, for instance, the cell cluster generation rate depending on the flow instability on the meso-scale DSI, or the convectively available potential energy (CAPE) on the synoptic scale. Similarly other model parameters, such as lifetime and size for cells and their clusters will be linked to the dynamic parameters.

Multiscale data and asymptotic model assimilation for atmospheric flows (A02)

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The atmosphere's multi-scale structure poses several major challenges in numerical weather prediction. One of these arises in the context of data assimilation. The large-scale dynamics of the atmosphere are balanced in the sense that acoustic or rapid internal wave oscillations generally come with negligibly small amplitudes. If triggered artificially, however, through inappropriate initialization or by data assimilation, such oscillations can have a detrimental effect on forecast quality as they interact with the moist aerothermodynamics of the atmosphere.

In the setting of sequential Bayesian data assimilation, we therefore investigate two different strategies to reduce these artificial oscillations induced by the analysis step. On the one hand, we develop a new modification for a local ensemble transform Kalman filter, which penalizes imbalances via a minimization problem. On the other hand, we modify the first steps of the subsequent forecast to push the ensemble members back to the slow evolution. We therefore propose the use of certain asymptotically consistent integrators that can blend between the balanced and the unbalanced evolution model seamlessly.

In our work, we furthermore present numerical results and performance of the proposed methods for two nonlinear ordinary differential equation models, where we can identify the different scales clearly. The first one is a Lorenz 96 model coupled with a wave equation. In this case the balance relation is linear and the imbalances are caused only by the localization of the filter. The second one is the elastic double pendulum where the balance relation itself is already highly nonlinear. In both cases the methods perform very well and could significantly reduce the imbalances and therefore increase the forecast quality of the slow variables.

Efficient calculation of slow and stationary scales in molecular dynamics (A04)

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Molecular dynamics (MD) simulation is a technique that aids in the understanding of fundamental processes in biology and chemistry, and has important technological applications in pharmacy, biotechnology, and nanotechnology. Many complex molecular processes have cascades of timescales spanning the range from 10^{-15} s to 1 s often with no pronounced gap that would permit efficient coarse-grained time integration. Essential information about the slow kinetic properties of macromolecules is contained in the eigenvalues and eigenfunctions of the dynamical operator of the molecular dynamics. To estimate these eigenfunctions, we have derived a variational principle that is based on the maximization of a Rayleigh coefficient [6]. We have shown that this Rayleigh coefficient can be estimated from statistical observables that can be obtained from short distributed simulations starting from different parts of state space. A suitable choice of basis functions is given by products of one-coordinate basis functions, which describe changes along internal molecular coordinates, such as dihedral angles or distances. We employ a sparse tensor product approach in order to avoid a combinatorial explosion of products [1]. Two typical strategies to simulate slow transitions such as protein conformational transitions or protein–ligand dissociation are (i) conducting large ensembles of short simulations and estimating the long-term kinetics with a Markov state model, or (ii) speeding up rare events by bias potentials or higher temperatures and estimating the unbiased thermodynamics with reweighting estimators. We have introduced the transition-based reweighting analysis method (TRAM), a statistically optimal approach that combines the best of both worlds and estimates a multiensemble Markov model (MEMM) with full thermodynamic and kinetic information at all simulated ensembles [4, 7, 8]. Using TRAM we have computed the full protein-ligand kinetics of the oncoprotein fragment $^{25-109}$Mdm2 and the nanomolar inhibitor peptide PMI. Using simulations with individual lengths of 1 microsecond and total simulation times of several 100 microseconds, we have predicted a dissociation time of seconds to tens of seconds, and have confirmed this prediction with experiments [2].

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An automatic adaptive importance sampling algorithm for molecular dynamics in reaction coordinates (A05)

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The poster shows a method we propose for adaptive importance sampling for dynamical quantities of high dimensional complex systems which are metastable. The main idea of this article is to combine a method coming from Molecular Dynamics Simulation, Metadynamics [1, 2], with a theorem from stochastic analysis, Girsanov's theorem [3]. The proposed algorithm has two advantages compared to a standard estimator of dynamic quantities: firstly, it is possible to produce estimators with a lower variance and, secondly, we can speed up the sampling. One of the main problems for building importance sampling schemes for metastable systems is to find the metastable region in order to manipulate the potential accordingly. Our method circumvents this problem by using an assimilated version of the Metadynamics algorithm and thus creates a non-equilibrium dynamics which is used to sample the equilibrium quantities.

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[3] B. Øksendal. *Stochastic Differential Equations: An Introduction with Applications*. Hochschultext / Universitext. Springer, Berlin, 2003.

Fault networks and scaling properties of deformation accumulation (B01)

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Well established explanations for earthquake activity in the lithosphere are based on strain accumulation and stress release along fault networks chiefly in plate boundary zones as described by rate and state dependent (RSD) friction models. Our goal is to derive, analyze, numerically approximate, and experimentally validate a multiscale model for fault networks consisting of a hierarchy of effective RSD models on increasing spatial and temporal scales.

As a first step, a variational one-body RSD model was developed and compared to an elastic slider on a rigid foundation through analogue experiments and numerical simulations. Furthermore, we established an experimental setup on the laboratory scale for studying strike-slip earthquakes using analogue models for single faults. Our novel, domain decomposition based approach to numerical homogenization of elliptic multiscale problems inspired two- and multilevel methods for linear model problems with coplanar fault networks.

From molecular dynamics to generalized Langevin dynamics to rate theories (B02)

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While the dynamics of complex molecules in water typically comprises many degrees of freedom, one is often only interested in a single observable, or even only the slowest time scale of the whole system. Thus, one often would like to project dynamics from a high-dimensional phase space onto a low-dimensional effective description, or even onto a single number. We study this coarse graining at the example of butane.

The slowest process in a butane molecule are dihedral angle reconfigurations, and starting from molecular dynamics (MD) simulations in explicit water we first show that the dynamics of the dihedral angle can be captured by the generalized Langevin equation. We do this by explicitly extracting the memory kernel, which describes non-Markovian effects of the projected dynamics, putting special emphasis on disentangling solvent effects from internal dynamics.

To extract time scales from the generalized Langevin equation, one typically employs a non-Markovian rate theory like the Grote–Hynes (GH) [1] or Pollak–Grabert–Hänggi (PGH) [2] theory. However, no systematic studies on how well these theories work exist. We compare direct simulations of the generalized Langevin equation with exponential memory to the predictions of the GH, PGH rate theories and find that GH theory only yields accurate predictions in the overdamped regime with short memory, while PGH theory works very well for all parameter regimes. We furthermore provide an easy-to-implement heuristic formula for rates as an alternative to the PGH formula, which is quite complex to implement.

Finally, we compare the rate-theory-predicted dihedral reorientation times to those extracted directly from MD simulations, validating our two-step coarse graining procedure.

[1] R. F. Grote and J. T. Hynes. The stable states picture of chemical reactions. II. Rate constants for condensed and gas phase reaction models. *The Journal of Chemical Physics*, 73(6):2715, 1980.
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Multilevel coarse graining of multiscale problems (B03)

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The advancement of computational power allows for the simulation of increasingly complex molecular systems. Still, the global analysis of such systems on long time scales and in all-atom detail remains out of reach due to the high dimension of the state space. The goal of coarse graining is thus to find a reduced description of the system which preserves the long-time dynamical properties with sufficient accuracy. We present a new characterization of good coarse graining coordinates and based on that novel techniques for the systematic derivation of reduced models. Also, large-scale biomolecular systems to which the newly-developed methods are applicable are discussed.

Tensor product decomposition methods applied to multi-scale data with self-similar characteristics (B04)

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Low-rank approximation methods are often suited to attack high-dimensional problems successfully and allow very compact representations of large data sets. Specifically, hierarchical tensor product decomposition methods emerge as an promising approach for application to data that are concerned with cascade-of-scales problems as, e.g., in turbulent fluid dynamics. Here, we focus on two particular objectives, that is representing turbulent data in an appropriate compact form and, secondly and as a long-term goal, finding self-similar vortex structures in multi-scale problems. The question here is whether tensor product methods can support the development of improved understanding of the multi-scale behavior and whether they are an improved starting point in the development of compact storage schemes for solutions of such problems relative to linear ansatz spaces. We discuss the challenges of our approach and present reconstruction capabilities of a tensor product decomposition based modeling approach tested against 3D turbulent channel flow data.

Markov state models with Girsanov reweighting (B05)

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Molecular Dynamics (MD) is characterized by metastable states and transitions that occur at different timescales. Recent studies [4] have proven, through Markov State Models (MSM) analysis, that the timescales are very sensitive on the potential energy function of the molecule and even small perturbations produce large effects on the dynamics of the system. We model the molecular dynamics by a Langevin equation, then we construct a MSM on the generated trajectory, whose transition probability matrix can be written in terms of the time correlation function:

$$C_{ij} = \mathbb{E}_P \left[\mathbf{1}_{A_i}(x_0) \mathbf{1}_{A_j}(x_t) \right]$$

where P is the path probability measure of the system, x_t is the trajectory and A_i are the sets of the conformational space. Because the potential energy perturbation affects the path probability measure of the system, we can exploit the Girsanov theorem [2] to evaluate the change of measure:

$$\frac{\mathrm{d}Q}{\mathrm{d}P} = \exp\left(-\int_0^t \frac{\nabla U(x_s)}{\sigma} \mathrm{d}B_s - \frac{1}{2} \int_0^t \left(\frac{\nabla U(x_s)}{\sigma} \right)^2 \mathrm{d}s \right)$$

where Q is the new path probability measure, $U(x)$ is the potential energy perturbation, B_t is a Brownian motion under probability measure P and σ is the volatility. This leads to redefine the time correlation function under the new path probability measure Q and to construct the MSM of the system under the perturbation $U(x)$ [1, 3].

The method can be used to predict the timescales of a molecular system without rerunning molecular dynamics simulation, when an external force is applied to the potential energy. In particular the method could be relevant to force-field optimization.

We performed tests of diffusive processes verifying the limits of applicability of the method. Then we have tested many-body systems in three-dimensional space, formulating an extension of the method when the MSM is constructed on a conformational space not directly perturbed. We present also results for alanine dipeptide and a benchmark test that shows the efficiency of the method.

This research is representative of the work realized within the project B05 that contributes to the SFB1114 by investigating the scaling cascades in protein dynamics from a mathematical point of view, by developing new mathematical tools to study Molecular Dynamics simulations and comparing numerical results to results from infrared spectroscopy.

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Adaptive coupling of scales in molecular dynamics simulations of complex molecules (C01)

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The Adaptive Resolution Simulation (AdResS) approach [2] allows the combination of molecular dynamics simulations of different resolution in different parts of the simulation box with particle-exchange through a transition region. This is accomplished by interpolating the interactions associated with different resolutions according to the position of the molecule in the transition region and correcting for disturbances caused by this transition through a localized thermostat and a correction force. While the method has been well established for small molecules like water, more complex molecules until now had to be restrained to remain in one region [3], allowing only the surrounding solvent to change resolution.

We have extended the method to be applicable to polymer liquids [1] and biomolecules. As an example, we are applying the method to lipid membranes, using both explicit solvent and implicit solvent models for the coarse grained region.

[1] J. H. Peters, R. Klein, and L. Delle Site. Simulation of macromolecular liquids with the adaptive resolution molecular dynamics technique. *Physical Review E*, 94(2):023309, Aug. 2016.
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[3] J. Zavadlav, R. Podgornik, and M. Praprotnik. Adaptive Resolution Simulation of a DNA Molecule in Salt Solution. *Journal of Chemical Theory and Computation*, Sept. 2015.

Markov state modeling for bulk water dynamics (C02)

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Water has always been of great interest of research. It is related to a large range of processes governing biological, chemical and physical applications. A prominent goal has been to connect the macroscopic behaviour to the microscopic structure and thus to the hydrogen bonds (H-bonds) between individual water molecules. Based on trajectories describing the relative position between pairs of water molecules obtained from MD simulations, different processes associated to H-bond breaking events are analyzed by a Markov state model. We find that the meta-stable states in the Markov state model are H-bonds where when mapping onto a transition matrix the eigenvectors describe breaking and forming of H-bonds. When adding an additonal water molecule to the Markov model the dynamics is still Markovian with the advantage that an H-bond switch from one to another molecule can be seen. The application of transiton path theory to the three-water molecule system reveals competing scenarios when an H-bond is broken and formed.

Multiscale modelling and simulation for spatio-temporal master equations (C03)

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Depending on the particle concentration and mobility, different mathematical models for chemical reaction kinetics are appropriate. Many biological processes require the high spatial and temporal resolution of particle-based models which are computationally demanding and call for efficient mathematical and numerical methods. This project aims at developing *high performance simulation tools* for particle-based dynamics as well as finding adequate model discretizations in terms of *spatial coarse-graining*. The relation between the different models is specified and a multiscale theory will be developed.

Effective models for interfaces with many scales (C05)

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Project C05 focuses on modeling and analysis of stationary and evolutionary problems in multiscale systems. The different scales may arise in space or in time. To this aim, we use techniques from thermodynamical modeling, i.e. the GENERIC, as well as variational methods and methods from stochastic homogenization. On our poster, we present five recent mathematical results of the project that go into these directions: A connection between gradient flows and large deviation principles obtained via evolutionary Γ-convergence, Global existence of solutions for a viscoplasticity model at finite strain, stochastic homogenization of rate-independent systems, time-averaging of oscillatory dissipation potentials and an application of stochastic homogenization to a convergence proof for a numerical scheme developed by M. Weber from Project A05.

Intensification of atmospheric vortices through asymmetric multiscale convection (C06)

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The dynamics of atmospheric vortices such as tropical storms, hurricanes and mid-latitude cyclones is driven by a variety of interacting scales. [1] developed an asymptotic theory for the dynamics of strongly tilted atmospheric vortices in the gradient-wind regime, embedded into a synoptic-scale geostrophic background field. One central outcome of the theory is the evolution equation for the nearly axisymmetric primary circulation. It predicts that Fourier-mode 1 of asymmetric diabatic heating/cooling patterns can spin up or spin down a vortex depending on the relative arrangement of the heating dipole relative to the vortex tilt. Up to this point the theory is restricted to dry air and externally imposed heating, and it neglects influences of the (turbulent) boundary layer.

On this poster we summarize two recent developments that aim at extending and consolidating this theory: The first part describes three-dimensional numerical simulations based on the pseudo-incompressible flow equations as implemented in the EULAG code [2]. These corroborate the asymptotic predictions nicely and show strong intensifications on the timescale of days.

The second part of the poster describes recent developments of a novel multiscale asymptotic regime that resolves the localized deep convective cloud towers thought to be responsible for the asymmetric heating patterns postulated in the vortex theory.

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Stochastic spatial coagulation processes (C08)

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We look at systems of stochastically reacting particles, including the case of coagulating–fragmenting particles. We study the situation where concentrations converge to solutions of a deterministic differential equation, the so-called reaction rate equation, as the number of particles goes to infinity. In particular, we study the large deviations, that is, the exponential rate of convergence of the probabilities in path space. The large deviations rate enables the study of fast–slow reaction limits, or the convergence of a reaction–diffusion PDE to a well-mixed ODE via Gamma-convergence techniques. In particular, for systems in chemical detailed balance, the large deviations induce a gradient structure, which can then be used to study fast diffusion or fast reaction limits via evolutionary Gamma-convergence.

Particles in lipid bilayers (AP01)

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A variety of models for the membrane-mediated interaction of particles in lipid membranes are considered in the literature. We present a consistent variational framework for the mathematical treatment of hybrid models for particle–membrane interaction. The framework allow to show existence and uniqueness results and embeds established and new models in a hierarchy of successively simplified models [1]. It is also the foundation for the development and rigorous numerical analysis of efficient unfitted finite element methods for particle–membrane problems with fixed lateral particle positions [2]. Using methods from shape-calculus allows to also treat particles that are moving and rotating in lateral direction via membrane-mediated mechanical interaction [3].

In the next steps we plan to bridge the hybrid models considered so far to more scales in several directions. On the one hand we will use the developed techniques to incorporate membrane-mediated mechanical interaction into smaller scale Brownian-motion approaches. On the other hand we want to exploit the developed understanding for hybrid models with discrete particles to derive larger scale continuum models for large particles numbers.

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Fullerene in water: Local microscopic structures vs. quantum delocalization of atoms in space

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We have performed molecular dynamics simulations of fullerene in water, where water molecules are treated using the path-integral formalism of Feynman. Path-integral molecular dynamics (PIMD) describes the quantum delocalization of light nuclei which may lead to different structure and dynamics of the hydrogen bonding network as compared to classical MD. We have employed the grand-canonical adaptive resolution simulation method (GC-AdResS) to identify the essential degrees of freedom required to reproduce a particular property. Using this method, we have shown that the water structure around solute is "local" irrespective of quantum or classical description of water molecule. However, it has been seen that the water structure around the solute is more flexible and disordered when one uses the quantum description. Following these results, we have proposed a model describing the aggregation process of fullerene molecules in water where nuclear quantum effects play an important role.

Comparison of recent physically-based stochastic subgrid-scale parameterizations

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Since the beginning of the century, various physically-based stochastic reduction methods have been developed in the context of climate modelling. The multiplicity of available stochastic parameterization approaches illustrates how fruitful was the seminal work of Hasselmann about it in the 1970s. However, in this perspective, one might wonder about their relative efficiency in different situations. Indeed, depending on the specific purpose that it needs to fulfill, some parameterizations might perform better than others. The present work aims to shed some light on these questions by illustrating these methods on a simple stochastic triad system relevant for the atmospheric and climate dynamics, and for which most of the calculations can be made analytically. We show in particular that the stability properties of the underlying dynamics of the subgrid-scale processes has a considerable impact on their performances.

Is DFT accurate enough for modeling chemical kinetics? Quantifying the error propagation in first principles models

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Targeting at an understanding of interplay between bond making and bond breaking and observed reactivity, first-principles based kinetic methodologies for heteroStructure Sensitivity of the Oxygen Evolution Reaction Catalyzed by Cobalt(II,III) Oxidegenous catalysis employ energetic information derived from electronic structure calculations. These energies, usually obtained on the density functional theory (DFT) level, have typically a potential error of 0.2–0.3 eV. We present a systematic approach to address the propagtion of these errors to the kinetic model's result based on adaptive sparse grids for the sampling of the error space. We demonstrate the approach on a model for the oxygen evolution on Co_3O_4 [1]. Our results indicate that the simulated reactivities carry an uncertainty of more than five orders of magnitude, questioning the trustability of the model. However, a decomposition of this uncertainty into contributions of different input errors reveals that only a small number of DFT energies have an impact. So, it is still possible to draw conclusions about the potential driving forces behind catalytic activity, although the activity itself can not be estimated accurately. Besides a qualified discussion of the effect of the modeling error, the approach can be employed for the reduction of the number of expensive first-principles simulations or for computational materials screening.

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A maximum entropy parameterization for the stochastically forced Burgers equation

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Due to limited computational power a common problem encountered in the simulation of complex phenomena covering wide range of scales is the representation of some unresolved processes. Such unresolved scales are typically parameterized by fitting some model of the resolved scales. Recently Verkley, Kalverla and Severijns (QJRMS, 2015) proposed an approach for parameterization of dynamical systems which does not require any fitting, but uses the maximum entropy principle from information theory. With this approach a probability density function (PDF) of the unresolved scales can be determined by imposing some constraints, e.g., by assuming vanishing averaged energy tendency. The maximum entropy principle allows to find the least biased PDF consistent with the information of the system. We apply the same approach to a stochastically forced system in the form of the Burgers equation. The resulting deterministic parameterization improves the spectrum of the resolved scales. It is compared with other approaches such as stochastic mode reduction, which require minimal regression fitting of the unresolved scales only.

Time scales in the cubic nonlinear Schrödinger equation

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Several time scales are important in nonlinear Schrödinger equations. On the one hand, high oscillations are introduced into the dynamics by the unbounded differential operator. On the other hand, some quantities are nearly preserved on long time intervals, and some quantities are even conserved for all times, most prominently the energy of this Hamiltonian partial differential equation. On the poster, some results on the behaviour of solutions on these time scales are described, and the corresponding behaviour of a typical (structure-preserving) numerical method on these time scales is discussed. This is based on joint work with Erwan Faou (Rennes) and Christian Lubich (Tübingen).

A systematic energy conserving algorithm for the stochastic 2-layer QG model

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We will systematically derive a stochastic version of the 2-layer quasi- geostrophic (QG) equations based on its Hamiltonian formulation. The stochastic terms will be introduced in such a way that the total energy is conserved. The barotropic and baroclinic modes will be separated through a parameter ϵ depending on the different time scales of the modes involved. Afterwards a stochastic mode reduction will be performed on the system, i.e. baroclinic mode will be eliminated and we will derive an effective model for only the barotropic mode. We will develop a suitable stochastic solver in such a fashion that the resulting numerical model will be energy conserving. In our presentation we will discuss the results.

Data assimilation in a fast-slow system of atmosphere

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Over the last few decades much progress has been made in improving data assimilation schemes. The assimilation of observations into operational prediction models greatly increases the predictiveskill of weather forecasts. Seasonal and decadal-scale prediction systems are coupled systems of two climate components: the slow ocean and the fast atmosphere. We use the conceptual Lorenz-96 two-level model to present the nonlinear and chaotic property of the real atmosphere. We formulate the two-level model in such a way that it contains a coupling term determining the time scale separation. Furthermore, we use deterministic and stochastic parametrization schemes to represent the evolution of the fast variables; which can also be interpreted as model error. The parametrization schemes only depend on the resolved slow variable. We call the model with such parametrization schemes a reduced model. The larger the time scale separation, the better the reduced model represents the full dynamic model. We perform the ensemble Kalman filter (EnKF) to the Lorenz-96 two-level model with different time scale separation. The accuracy of analysis has no obvious difference when ensemble size is sufficient. If we are only interested in predicting slow variables, then assimilating observations into evolution of fast variables is not necessary. Comparison between full dynamic model and reduced model shows that accuracy of analysis slightly improved when apply EnKF to reduced model. Reduced model with autoregressive process of higher order performs better than with first order autoregressive process in terms of predictive skill. This result is obivous when time scale separation is large. As the time scale separation decreases, the difference disappers. We will also discuss how well the analysis represent extreme events and whether the implementation of EnKF influence the occurrence of extreme events.

Grand canonical adaptive resolution simulations, optimal control, and Markov State Models (Towards open boundary simulations)

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Ionic liquids are one of the most challenging systems in physical chemistry. Theoretical work has shown a counterintuitive characteristic that is a large class of ionic liquids is characterized by local scale. However, several basic properties are still unknown and unpredictable. From the theoretical point of view ILs present a challenge for simulations with open boundaries. The challenging aspect in particular is how to build a reservoir of charged particles and the minimum requirements for the coarse grained model.

We perform Grand Canonical-like Adaptive Resolution Simulations of Dimethyl-imidazolium chloride as a basic example for ionic liquids and a stepping stone for further and more complex systems. In our work we propose two different coarse-graining potentials and determine several properties as a check for the validity of our ansatz. Results are highly satisfactory.

The work has been published in [1].

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Scaling transdisciplinary cascades of potential side effects of stratospheric aerosol injection

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Climate change is a fundamental challenge for humankind. The deployment of climate engineering (CE) technologies is discussed as one of the possible solutions if mitigation fails or to support mitigation efforts to reach the goal of staying below the target of 1.5 to 2° C global temperature increase, as agreed in the Paris Treaty. Among CE technologies, stratospheric aerosol injection (SAI) is considered to be one of the most risky solutions because of its large amount of potential side effects. Thus, it is especially important to analyze, how "risky" it actually is – considering not only potential pollution effects in natural systems, biodiversity, or the physical termination effect, but also potential social implications such as on societal stability or conflict.

To assess this question we assign equations to the s chematic overview of possible consequences of the deployment of SAI (stratospheric aerosol injection) ([1, p. 71]) that quantify all interactions. We implement this information in a diffusion model to visualize and scale transdisciplinary cascades and potential sinks in the transdisciplinary network of chains of side effects. Furthermore, we analyze selected pathways of causal relations to emphasize the role of feedback processes in this complex reaction system

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A computationally efficient stochastic model of atmospheric cumulus convection

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Most convection parameterization schemes currently used within numerical weather prediction (NWP) models assume that the convective response of an individual model grid box is in equilibrium with the convective forcing at each time step. The resolution of many NWP models is already finer than the resolution at which this equilibrium assumption is fulfilled (horizontal mess size is less than 50 km). As the convective response is not necessarily in equilibrium with the large-scale forcing, fluctuations of convection-related quantities about their equilibrium values should be accounted for. To describe these fluctuations, e.g. fluctuations of the mass flux at the cloud base, stochastic convection schemes have been developed for both deep (Plant & Craig 2008) and shallow (Sakradzija & Seifert 2015) convection. Both schemes deal with an explicit representation of the set of clouds which may emerge and disappear according to certain statistical laws, that are partially derived analytically from some basic assumptions and partially based on results from LES and cloud-resolving model simulations. Due to the need to explicitly track individual clouds following their lifecycle, these schemes can be computationally expensive. Furthermore, the information the schemes contain is to some extent redundant as only the total mass flux of all living clouds is required for the host atmospheric model. Motivated by the above considerations, the present authors attempted to reduce the machinery of the above schemes to the solution of only two first-order stochastic differential equations, namely, the equations for the number of living clouds N and for the sum of their mass fluxes at the cloud base M. The equations are tailored in a way that the behaviour of the quantities in question is equivalent to their behaviour in the original schemes. It is demonstrated that, if the lifetime of all clouds is the same and constant (as is the case for the Plant & Craig scheme), it is impossible to develop stochastic differential equations capable of describing the stochastic processes for N and M identical to the respective processes in the original convection schemes. However, a modified formulation, where an exponential distribution of the cloud lifetimes is assumed, yields a completely identical solution. It is shown that, although this modification seems to be quite significant, the differences in the properties of N and M between the original and modified formulations are small and clearly acceptable for practical purposes. It seems impossible to derive stochastic differential equations for N and M which identically reproduce the shallow convection scheme of Sakradzija & Seifert. However, a solution is obtained which recovers the original-scheme solution to a very good approximation. A general approach to reduce a stochastic cloud scheme with an arbitrary distribution of the mass fluxes of individual clouds and with an arbitrary dependence of the cloud lifetimes on their mass fluxes is presented.

Estimating parameter gradients from stochastic simulation of complex reaction networks

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We present a three-step procedure for the sampling of local sensitivities (parameter gradients) from stochastic simulation [2], which severely reduces the computational costs compared with standard numerical differentiation. In the first step, we utilize the Relative Entropy Method [4] for obtaining upper/lower bounds for the derivatives and discard those parameters with vanishing sensitivity. For the remaining, we sample the derivatives from a single trajectory employing an estimator based on Linear Response Theory. It turns out that some sensitivities can very well be sampled, while others show a higher variance. Only for the later, we perform a numerical differentiation using Coupled Finite Differences (CFD) [1]. We demonstrate the approach on a on the CO oxidation on the RuO2(110) surface [3]. We find that CFD is only necessary for a small fraction of the sensitivities.

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Riemannian optimization in tensor train format

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Problems of very high dimensions have recently encouraged the development of tensor decomposition formats such as the Tensor Train (TT) format. It has been established that tensors of fixed (low) TT-rank form a manifold. This fact can be exploited for optimization. We have developed several Riemannian Optimization schemes and we compare their performance. An idea for rank adaptivity is given.

Analysis on clouds and geostrophic wind effects on regime occupation statistics in nocturnal boundary layer

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Turbulence is the main process responsible for the exchange of the energy, momentum and mass between the Eerth surface and the atmospheric boundary layer (ABL). More specifically, the transfer of moisture drives cloud formation in the ABL. During daytime, the buoyant plumes, driven by the convective radiative transfer, are the main source for moisture transfer into the boundary layer, and consequently possible cloud formation. The wind shear-driven turbulence however, is an important factor in triggering formation and evolution of nocturnal boundary layer (NBL) stratus, when only long-wave radiative cooling is present. As a part of the High Definition Cloud and Precipitation (HD(CP)^2) project, this study aims to contribute in better understanding of the NBL turbulence and clouds interaction. By using high resolution meteorological and clouds data from supersites (e.g., JOYCE – Jülich ObservatorY for Cloud Evolution), and applying to a data-driven statistical clustering method, we are analyzing the affects of cloud presence and geostrophic wind on regime occupation statistics. Presented results are discussed.

Adaptive tsunami simulations with RKDG schemes on triangular grids

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Due to their potentially disastrous impact on environment and society the numerical simulation of tsunami events demands for accurate and effi- cient algorithms. In this presentation, two important aspects in this respect are discussed: dynamic mesh adaptivity and the treatment of inundation at the coast.

The multiscale nature of a tsunami event promotes the application of adaptive grid algorithms. In the beginning, when the tsunami has just been generated by an earthquake, an accurate solution is only needed near the source in the deep ocean. During the propagation of the tsunami wave across the ocean, the domain of influence spreads, and the computational grid must be adapted. In the final phase, when the tsunami wave inundates the coast, accurate solutions are of most interest in highly populated areas. For realistic simulations, these often have to go down the scale of meters. In the presented framework the adaptive grid generator amatos is applied, which uses triangular grids and a bisection-based refinement strategy. A local error indicator controls the adaptivity of the grid. For the numerical modeling of the tsunami event a Runge–Kutta discontinuous Galerkin (RKDG) discretization of the shallow water equations is employed. The proposed algorithm preserves the steady state of a fluid at rest, is mass conservative and preserves the positivity of the fluid depth. The novel wetting-and-drying treatment is based on a limiting approach. The core of the method is a velocity based "limiting" of the momentum, which provides stable and accurate solutions in the computation of wetting and drying events.

The performance of the method is verified by several analytical test cases and is finally applied to realistic tsunami test problems.

A proof of concept for scale-adaptive parameterizations: The case of the Lorenz '96 model

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Constructing efficient and accurate parameterizations of subgridscale processes is a central area of interest in the numerical modelling of geophysical fluids. Using a modified version of the two-level Lorenz '96 model, we present here a proof of concept of a scale-adaptive parameterization constructed using statistical mechanical arguments. By a suitable use of the Ruelle response theory, it is possible to derive explicitly a parameterization for the fast variables that translates into deterministic, stochastic and non-markovian contributions to the equations on motion of the variables of interest. We show how the parameterization is computationally parsimonious and has great flexibility, as it is explicitly scale-adaptive, and we prove that it is competitive versus empirical ad-hoc approaches.

Local stochastic subgrid-scale modeling for a one dimensional shallow water model using stochastic mode reduction

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Due to the finite spatial resolution in numerical atmospheric models, subgrid-scale (SGS) processes arise. This leads to an SGS error which also influences the resolved modes. Therefore a parameterization of these excluded processes might improve the model on all scales. In this study we present a model derived parameterization of these processes for the one dimensional shallow water equations.

To parameterize the SGS processes we choose the MTV stochastic mode reduction [2]. For this the model is separated into fast and slow processes. Then using the statistics of the fast processes, a SGS parameterization is found. To identify fast processes the state vector of the model is separated into two state vectors. One vector is the spatial average of the full model state vector in a coarse grid cell. The other, which describes SGS processes, is defined as the deviation of the full state vector from the coarse cell average. If the SGS vector decorrelates faster in time than the coarse grid vector, the stochastic MTV SGS parameterization can be derived from the model equation, which is the advantage of this method compared to others. So far the method was successfully applied on the Burgers-equation [1].

To apply the method onto the one dimensional shallow water equations, we choose a local approach of the fine variable self-interactions. With this, we are able to derive a local SGS parameterization using MTV's method leading to a closed model wrt. the coarse variable. We show, that this model is able to fix the energy decrease for high wave numbers which appears at the coarse resolution model with neglected SGS parameterization.

In the future we plan to extend the model to two dimensions and multiple layers. Perspectively, the method can be used to derive a stochastic SGS parameterization for the Navier-Stokes equations.

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