Universität Hamburg
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CSE Workshop 2025

Neumünster, April 2-4, 2025

Book of Abstracts

Organizing Committee:

Jörn Behrens (UHH)
Claudine von Hallern (UHH)

Program Committee:

Jörn Behrens (UHH)
Malte Braack (CAU)
Armin Iske (UHH)
Sabine Le Borne (TUHH)
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Thomas Slawig (CAU)

We gratefully acknowledge support from

Research Training Group GRK 2583, funded by DFG, as well as Kiel University

GRK 2583

Kiel University
Christian-Albrechts-Universität zu Kiel

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Program

Time	Wednesday, April 2	Thursday, April 3	Friday, April 4
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10:40-11:15	A. Rösler	Coffee	Coffee
11:15-11:40	K. Firdaus	M. Braack	O. Marx
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12:05-12:30	M. Ann	P.Schulz	A. Baksi
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Wednesday, April 2, 2025

Andreas Rößler (U Lübeck): Numerical treatment of SPDEs - a challenge for higher order approximations

Abstract: We consider the problem of approximating mild solutions of stochastic evolution equations driven by a Q-Wiener process. Therefore, an infinite dimensional version of a higher order derivative-free Milstein type scheme for the time discretization is proposed. For example, the introduced scheme can be applied to a certain class of semilinear stochastic partial differential equations (SPDEs) with commutative as well as non-commutative noise. In case of non-commutative noise, iterated stochastic integrals of the driving Q-Wiener process have to approximated. Finally, the order of convergence and the efficiency of the new scheme will be discussed.

This is joint work with C. von Hallern, University of Hamburg (UHH)

Kemal Firdaus (UHH): Locally Adaptive Non-Hydrostatic Model for Solving Moving Bottom-Generated Waves

Abstract: This research proposes a locally adaptive non-hydrostatic model and applies it to moving bottom-generated waves. This model is built upon the shallow water equations (SWE) extension with a quadratic pressure relation, which was proven to be equivalent to the Green-Naghdi equations, making it suitable for weakly dispersive waves. This extension has recently been improved so that it can be applied to waves generated from moving bottoms and manipulated in such a way that it can be solved by the projection-based method. However, this new set of equations still requires us to solve a system of elliptic equations over the entire computational domain at each time step, which demands more computational resources. Therefore, we develop an adaptive model that can reduce the computational time by solving the elliptic equations only in areas where dispersive effects might play a crucial role. To define these areas, we investigate several potential criteria based on the hydrostatic SWE solutions. We show that we can achieve a similar accuracy to the global adaptation with such a simple criterion, which reduces the computational time.

Thomas Slawig (CAU): Prediction of steady states in a marine ecosystem model by a machine learning technique

Abstract: We used pre-computed steady states obtained by a spin-up for a global marine ecosystem model as training data to build a mapping from the small number of biogeochemical model parameters onto the three-dimensional converged steady annual cycle. The mapping was realized by a conditional variational autoencoder (CVAE) with mass-correction. Applied for test data, we show that the obtained prediction by the CVAE already gives a reasonable good approximation of the steady states obtained by a regular spin-up. However, the predictions do not reach the same level of annual periodicity as obtained in the original spin-up data. Thus, we took the predictions as initial values for a spin-up. We could show that the number of necessary iterations, corresponding to model years, to reach a prescribed stopping criterion in the spin-up could be significantly reduced compared to the use of the originally uniform, constant initial value. The amount of reduction depends on the applied stopping criterion measuring the periodicity of the solution. The savings in needed iterations and, thus, computing time for the spin-up ranges from 50 to 95%, depending on the stopping criterion for the spin-up. We compared these results to the use of the mean of the training data as initial value. We found out that this also accelerates the spin-up, but only by a much lower factor.

Maša Ann (UHH): Dynamical Mode Decomposition of Extreme Events

Abstract: Most data-driven methods, among them Dynamical Mode Decomposition (DMD), focus on analysing and reconstructing the average behavior of a system. However, the primary interest often lies in the anomalous behaviour, known as extreme events. This is especially the case in climate

research, where extreme events have significant economic and societal costs. Therefore, we extend DMD method to account for extreme events by adding a penalisation term. This extension allows us to not only better reconstruct the extreme events, but also extract the spatial-temporal structures related to those extreme events. DMD was originally developed by Schmid ([1]) to enable the fluid dynamics community to identify spatio-temporal coherent structures (called modes) from high-dimensional data. In its essence DMD uses most relevant modes to filter the noise and reconstruct the original signal. We ask "Is the noise really noise"? Or can we attribute some of these dynamic modes, that result from the DMD, to extreme events? We applied this new method to the climate system, well known for its high-dimensionality. We examined two heatwaves that occurred in Europe (HW 2003 and HW 2010). In both cases we were able to improve the accuracy of the reconstruction. This novel variation of the DMD, can also be applied to other dynamical systems across many disciplines, in which extreme events are of interest.

[1] Joern Sesterhenn Peter Schmid. On dynamic mode decomposition: Theory and applications. 61st Annual Meeting of the APS Division of Fluid Dynamics, 53(15):391–421, 2008.

Joshua Lampert (UHH): Challenges and opportunities of using summation-by-parts operators with radial basis functions

Abstract: Entropy stability is a foundation of numerical methods for hyperbolic conservation laws, thereby ensuring the stability and robustness of the resulting numerical solutions. Summation-by-parts (SBP) operators provide a general framework to systematically develop entropy-stable schemes by mimicking continuous properties on a discrete level. They have proven to be a powerful tool to provide stable and high-order accurate numerical solutions. Classically, they are developed in order to differentiate polynomials up to a certain degree exactly. However, in many cases alternative function spaces are more appropriate to approximate the underlying solution space. One class of promising functions are radial basis functions (RBFs). Especially in multidimensional problems with potentially complex domains RBFs are known to possess very good approximation properties. However, applying classical RBF methods to hyperbolic problems often leads to stability issues. By combining RBFs with SBP operators, we can obtain provably entropy-stable discretizations in a mesh-free setting.

This talk discusses properties of multidimensional function space SBP (MFSBP) operators and presents an optimization-based construction procedure based on a recently proposed one-dimensional algorithm. The algorithm allows arbitrary function spaces and node distributions. I discuss some challenges and opportunities of the approach and show some preliminary results for using MFSBP operators to solve hyperbolic conservation laws.

Michael Koch (TUHH): Discretizing the Steady State Oseen Equations in An RBF-FD Setting

Abstract: The Radial basis function finite difference (RBF-FD) method has recently emerged as an alternative to classical finite difference or finite element discretizations of (systems) of partial differential equations. After a brief introduction to the RBF-FD method, it is described how to discretize the steady state Oseen equations in an RBF-FD setting. Furthermore different approaches to deal with the pressure constraint are presented and compared. In our numerical results, we focus on RBF-FD discretizations based on polyharmonic splines (PHS) with polynomial augmentation. We illustrate the convergence of the method for different degrees of polynomial augmentation, viscosities and domains. In particular it is shown why the error in the velocity increases inversely proportional to the viscosity.

Max Lewerenz (UHH): Kernel Based Reconstruction in Magnetic Particle Imaging

Abstract: This master's thesis presents a novel approach to image reconstruction in magnetic particle imaging (MPI). MPI is a tomographic imaging technique that emerged in 2005, leveraging magnetic fields for the visualization of ferromagnetic tracer materials.

The generalized Hermite-Birkhoff interpolation method provides a flexible framework for all sorts of interpolation problems. Following kernel-based reconstruction techniques as proposed by De Marchi, Iske, and Sironi in the context of computed tomography, this thesis adapts these principles to the MPI framework, aiming to enhance image reconstruction capabilities.

Despite applying the kernel-based reconstruction method to MPI, the formulation encountered challenges that prevented the establishment of analytical representations for elements in the interpolation space and the reconstruction matrix entries. To address these issues, discretizations were implemented, aligning efforts with the ultimate goal of developing a kernel-based reconstruction technique in MPI. The proposed method has the advantage that it delivers continuous solutions to the interpolation problem that can be evaluated in arbitrary positions of the field of view, not only in the grid inherent to the experiment conducted in the scanner.

The developed method still has one critical limitation: the necessity for grid-structured data points of known system functions. To overcome this barrier, an interpolated kernel-based reconstruction approach is introduced, allowing for the reconstruction to be performed at arbitrarily selected evaluation points while accommodating scattered data. This method preserves the advantages associated with kernel-based reconstruction, broadening its applicability and allowing for scattered samples of the scanner's system functions.

The proposed techniques have been implemented in the julia programming language, with experiments conducted using the real-world "OpenMPIData" as well as a modeled phantom and system matrix.

Faranak Gholampour (UHH): On the Approximation Order of Kernel-Based Cell Average Reconstruction in Finite Volume Methods

Abstract: Radial basis kernels can be used to recover cell average data in finite volume methods for solving conservation laws. This paper derives the convergence rates for cell average reconstruction based on (conditionally) positive definite kernels. We focus on error estimates for functions from the associated native space of the basis function of interest. To this end, the generalization of local polynomial reproduction and power functions for cell average reconstruction will be discussed. Finally, we provide error estimates in terms of cell size for some popular radial basis functions.

Stefan Turek (TU Dortmund): Hardware-oriented Numerics for Massively Parallel & Low Precision Accelerator Hardware and Application to „large scale" CFD Problems

Abstract: The aim of this talk is to present and to discuss how modern High Performance Computing (HPC) facilities including massively parallel hardware with millions of cores together with very fast, but lower precision accelerator hardware can be exploited via techniques from hardware-oriented Numerics for PDEs so that a very high computational and numerical efficiency can be obtained. Here, as prototypical large scale PDE-based applications, we concentrate on nonstationary flow simulations with hundreds of millions or even billions of spatial unknowns in long-time computations with many thousands up to millions of time steps. For the expected huge computational ressources in the coming exascale era, such spatially discretized problems which typically are treated sequentially in time, that means one time step after the other, are still too small to exploit adequately the huge number of compute nodes, resp., cores so that further parallelism, for instance w.r.t. time, might get necessary. In this context, we discuss how "parallel-in-space global-in-time" Newton-Krylov Multigrid

approaches can be designed which allow a much higher degree of parallelism. Moreover, to exploit current accelerator hardware in lower precision (for instance, GPUs), that means mainly working in single or even half precision, we discuss the concept of "prehandling" (in contrast to "preconditioning") of the corresponding ill-conditioned systems of equations, for instance arising from Poisson-like problems in incompressible flow simulations.

Here, we assume a transformation into an equivalent linear system with similar sparsity but with much lower condition numbers so that the use of lower precision hardware might get feasible. In our talk, we provide for both aspects numerical results as "proof-of-concept" and discuss the challenges, particularly for large scale flow problems.

Thursday, April 3, 2025

Josefin Ahlkrona (Stockholm Univ.): Numerical Methods for simulations of Ice Sheets and the surrounding Ocean

Co-Authors: André Löfgren, Lukas Lundgren, Clara Henry, Igor Tominec

Abstract: This talk presents our work on finite element methods for ice-sheet simulations, with a particular focus on numerically stable time-stepping schemes. A major challenge in ice-sheet modeling is numerical instability, which imposes restrictions on time step sizes and, consequently, computational efficiency. We introduce a method that significantly increases the largest stable time step, enabling substantial speed-ups in simulations. Our approach retains the stability benefits of implicit solvers while maintaining a computational cost per time step close to that of explicit solvers. This improvement stems from enhanced coupling between the equations governing geometry evolution and momentum balance. The improved stability facilitate the use of higher-order physics models, which are especially critical in coastal regions where ice sheets interact with the ocean. In the end of this talk, we explore some challenges in modeling ice in contact with the ocean and present some simulations of meltwater-driven ocean circulation near ice sheets.

Jost Kemper (CAU): Modeling Oceanic Flow in OpenFOAM with Application to Marine CDR Technologies

Abstract: Marine Carbon Dioxide Removal (CDR) options are currently actively explored due to their considerable potential to offset anthropogenic residual emissions and thus contribute to the net-zero carbon emission targets set out by numerous governments.

To model buoyant oceanic flows and turbulent mixing of tracers in the context of marine CDR, we have developed a RANS-based Finite Volume solver using the OpenFOAM environment.

The new method solves a Boussinesq-type set of fundamental equations, including transport equations for passive and active tracers. Special emphasis is placed on turbulent scalar fluxes in buoyant oceanic flow and the influence of surface waves. We present several new developments, including an interface tracking method for free surface waves. Applications to trajectories and mixing of buoyant surface plumes in the context of the marine CDR method Artificial Ocean Upwelling are shown.

Rodrigo Cifuentes Lobos (UHH): Obtaining coseismic deformation from surface ocean currents in a flat bottom ocean

Abstract: During an earthquake, the coseismic deformation of the ocean floor is transmitted through the water column. If the earthquake’s energy is sufficiently large, it can uplift the ocean surface, and the subsequent collapse due to gravity leads to the propagation of waves as a tsunami. This perturbation also creates current fields, as water is pushed away from the uplifted area which carry information about the seafloor deformation, including its rate and distribution. By measuring the surface current fields, information about the earthquake’s underwater spatial and temporal part characteristics can be obtainable. Using data measured directly above the source, in conjunction with onshore measurements, may lead to better resolution of the inverted seismic source, especially near the shallower parts of the rupture, complementing traditional inversion methods, such as geodetic, tsunami waveform and seismic data based models.

As a first step, this work presents a method for inverting the sea surface current field induced by coseismic deformation, isolated from background currents such as tidal or wind-driven currents, to determine the distribution of deformation at the sea bottom, assuming a flat ocean floor and instantaneous deformation. We use a simple linear fluid model to relate the coseismic effects to surface ocean currents and test robust inversion methods, assessing the associated uncertainties,

using synthetic data and, as a benchmark, the deformation distribution from the 8.8 2010 Mw Maule earthquake. This approach offers novel insights into the use of new datasets for retrieving seismic source information.

Malte Braack (CAU): Mapped coercivity for the stationary Navier-Stokes equations and their finite element approximations

Abstract: This work addresses the challenge of proving the existence of solutions for nonlinear equations in Banach spaces, focusing on the Navier-Stokes equations and discretizations of thom. Traditional methods, such as monotonicity-based approaches and fixed-point theorems, often face limitations in handling general nonlinear operators or finite element discretizations. A novel concept, mapped coercivity, provides a unifying framework to analyze nonlinear operators through a continuous mapping. We apply these ideas to saddle-point problems in Banach spaces, emphasizing both infinite-dimensional formulations and finite element discretizations.

Our analysis includes stabilization techniques to restore coercivity in finite-dimensional settings, ensuring stability and existence of solutions. For linear problems, we explore the relationship between the inf-sup condition and mapped coercivity, using the Stokes equation as a case study.

For nonlinear saddle-point systems, we extend the framework to mapped coercivity via surjective mappings, enabling concise proofs of existence of solutions for various stabilized Navier-Stokes finite element methods. These include Brezzi-Pitkäranta, a simple variant, and local projection stabilization (LPS) techniques, with extensions to convection-dominant flows.

The proposed methodology offers a robust tool for analyzing nonlinear PDEs and their discretizations, bypassing traditional decompositions and providing a foundation for future developments in computational fluid dynamics.

Lina Fesefeldt (TUHH): Acceleration of Newton's Method in Structural Mechanics with p-FEM Initializations

Abstract: We consider displacement problems in structural mechanics using a hyperelastic material model. Newton's method is applied to obtain a linearized problem. The convergence of Newton's method depends strongly on the choice of the initial guess. In the case of divergence, load steps can be used to stabilize the method: The force acting on the body is applied incrementally, and each solution to the sub-problems serves as a new starting vector for the next load step. Although this method is intuitive and well established, it is also computationally and memory intensive. Using a benchmark problem from computational mechanics, we show how the computational effort can be reduced if the p-version of the FEM is used. We utilize the hierarchical structure of the high-order FE problem to efficiently construct initial vectors for Newton's method.

Pia Schulz (Uni Lübeck): Image Registration for a Dynamic Breathing Model

Abstract: Respiratory surface electromyography measures the electrical muscle activity during breathing non-invasively. Electrophysiological modeling of the respiratory cycle is a valuable tool for analysis of the signals. A promising approach for dynamic simulations is based on knowing the deformation of the torso at a finite number of time steps between expiration and inspiration. In order to provide a foundation for such models, we present a new image registration method that determines the torso transformation during the respiratory cycle. For this purpose, we extend a ResNet-LDDMM based 3D/3D registration approach. We modify the network structure and add 2D data taken during respiration into the registration to include information about the breathing motion. Our experiments show that these modifications improve the registration quality, thereby providing a step towards a more realistic model of electrical transfer behavior over the respiratory cycle.

Vamika Rathi (TUHH): Maxey-Riley-Gatignol Equations for Tracking Lagrangian Devices in Chemical Reactors

Abstract: The Maxey-Riley-Gatignol equations (MaRGe) are used to describe the motion of small, spherical inertial particles in fluids. They model the sparse concentration of inertial particles in a wide range of environmental, industrial, and geophysical processes, such as the dispersion of the COVID-19 virus, movement of particles in chemical reactors, and cloud formation. MaRGe are integro-differential equations due to the presence of the history force term, which is an integral term that makes them difficult and computationally expensive to solve. Most researchers neglect the history force; however, recent studies show that this term has a significant effect not only on the trajectories of individual particles but also on their larger-scale Lagrangian dynamics.

In my talk, I will present a numerical solver for the 3D MaRGe using quadrature schemes as proposed by Daitche (2013). Further, I will adopt techniques from the paper by Candelier et al. (2004) to derive an analytical solution for a 3D vortex as a test case. Finally, I will show results where we attempt to track simulated particles using an alpha-beta-gamma filter modified to use a simplified version of MaRGe as prediction model instead of the commonly used assumption of constant acceleration over a time step.

Finn Luca Sommer (TUHH): Universal differential equations for the Maxey-Riley equations

Abstract: Universal differential equations (UDEs) form a bridge between classical physical modeling and data-driven approaches from machine learning. An approach will be presented on how UDEs can be used to model the movement of spherical particles in a flow field.

For this purpose, the system of ordinary integro-differential equations known as Maxey-Riley-Gatignol equations is used. They model the movement of inertial particles in a fluid under the assumption that the movement of the particle does not influence the flow. This assumption is valid if the particle is sufficiently small. The integral term in the model makes it difficult to solve this equation using classical numerical methods, which is why it is often neglected in practice. However, since this can lead to qualitatively different solutions and thus to significant deviations from the actual solution even in simple flow fields, we propose to approximate it by a neural network, trained using reference trajectories.

We will analyze both the deviations of trajectories of individual particles and the values of the Finite-Time Lyapunov Exponent (FTLE). The results show that replacing the integral term by UDEs can result in quantitatively and qualitatively accurate approximations to the full model. Finally, possible extensions are discussed, such as the use of different network architectures..

Lütfiye Masur (UHH): Swift-Hohenberg equation with non-smooth nonlinearity

Abstract: The Swift Hohenberg equation is conceptual order-parameter model for structure formation in broad generality including fluid dynamics, in particular convection. It entails polynomial force terms, and I replace the monomials with general powers $|u|^a$, for which the bifurcation analysis has not been done. Such terms are motivated by non-smooth hydrodynamic forces and models of ship maneuvering, shimmying wheel. Due to these non-smooth terms, the analysis cannot rely on direct Taylor expansion. Numerical studies show intruiging behaviour of the periodic roll-type solution of Swift Hohenberg equation and of the homoclinic snaking (of solutions corresponding to convectons), which is a back and forth oscillations in the bifurcation diagram

Friday, April 4, 2025

Martin Gander (UNIGE): Parallel in Time Methods for Parabolic and Hyperbolic Problems

Abstract: Space-time parallel methods, also known more recently under the name PinT (Parallel in Time) methods, have a long history, but they have received a lot of attention over the past two decades. This is driven by the parallel hardware architectures that have now millions of cores, leading to saturation when parallelizing in space only. Parallelizing also the time direction is tempting, but this is very different from the space direction, because evolution problems satisfy a causality principle: the future is dependent on the past, and not the other way round.

I will show in my presentation that successful strategies for PinT methods depend strongly on the nature of the evolution problem. For hyperbolic problems, effective PinT methods are Domain Decomposition methods of Waveform Relaxation type, culminating in Unmapped Tent Pitching methods, ParaDiag methods, and also direct time parallel methods like ParaExp. Most of these methods can also be very effectively used for parabolic problems, but for such problems there are also highly successful multilevel methods, like Parareal and its variants. The currently best ones are however space-time multigrid methods. All these multilevel methods struggle however when applied to hyperbolic problems.

Henrik Wyschka (UHH): Numerical Solution of p-Laplace Problems for Shape Optimization

Abstract: Shape optimization constrained to partial differential equations is a vibrant field of research with high relevance for industrial-grade applications. Recent developments suggest that using a p-harmonic approach to determine descent directions is superior to classical Hilbert space methods. This applies in particular to the representation of kinks and corners in occurring shapes. However, the approach requires the efficient solution of a p-Laplace problem in each descent step. Therefore, we extend an algorithm based on an interior-point method without resorting to homotopy techniques for high orders p. Further, we discuss modifications for the limit setting.

A key challenge in this regard is that the Lipschitz deformations obtained as solutions in limit setting are in general non-unique. Thus, we focus on solutions which are in a sense limits to solutions for finite p and aim to preserve mesh quality throughout the optimization. Building upon this work, we also aim to reduce the number of outer iterations and thus calls of the algorithm by proposing a trust-region method. Due to the structure of the algorithm for finite p, we are able to introduce a constraint on the gradient of the solution naturally. Consequently, the obtained deformation fields also fulfill a trust-radius in terms of the Lipschitz topology.

Hanna Bartel (UHH): Multidimensional Opinion Formation

Abstract: Existing research on modeling opinion dynamics primarily examines scenarios in which individuals have opinions on only one topic. This talk presents a possibility of modeling opinion dynamics when individuals have opinions on multiple topics. I will introduce a kinetic model that describes the effect of interactions between people on their opinions, and discuss the corresponding partial differential equation, which describes that behavior on a macroscopic level.

Oliver Marx (UHH): Modelling and simulation of air flow dynamics inside termite mounds

Abstract: Termite mounds are complex animal-built structures with varied architectural designs depending on the species and respective habitats. One key function is to provide ventilation for the underground nest. This regulates the temperature of the nest and diffuses the metabolic gases

produced inside. A one-dimensional mathematical model is presented that describes the airflow dynamics within a termite mound. It is derived from the Euler equations of gas dynamics. A low Mach number asymptotic analysis is performed. Numerical simulation results are shown.

Ingenuin Gasser (UHH): MSO for renewable energy production

Abstract: We present new mathematical models used to describe power stations driven by renewable energies. This refers to solar thermal power, geothermic power, osmotic power etc. After setting up the models we run simulations. The final goal is the optimisation of certain crucial quantities such as the net power output.

Aditya Baksi (IAP): Atmospheric turbulence with energy sources at two disparate length-scales.

Abstract: High-resolution mesoscale model simulations demonstrate that convective systems are able to generate a kinetic energy spectrum with a slope close to -5/3. We compare such meteorological models to idealized non-hydrostatic dry Boussinesq turbulence simulations with triply-periodic geometry, where such results are generally not obtained. To make it analogous to a typical meteorological model, we configure our simulations by using similar model configurations. A first set of simulations took initial conditions as random buoyancy perturbations centered on an intermediate horizontal wavenumber. This caused a downscale cascade of energy, while producing a decaying peak that remained at the injection wavenumber. We were later able to produce the -5/3 spectral slope by specifying the initial buoyancy field as a series of aligned, localized structures, as used in previous meteorological studies (e.g, Sun et al., 2019). These structures produced a short-lived upscale transfer of energy. We also find that similar dynamics observed in meteorological models are somewhat robust to the grid aspect ratio.

Cancelled: Claudine von Hallern (UHH): On the Numerical Approximation of SPDEs in Geosciences

Abstract: Stochastic partial differential equations are a powerful tool to model various phenomena in the ocean or atmosphere. Since analytical solutions to these equations are, in general, not computable, there is a high demand for numerical schemes to approximate these processes. In this talk, we give a short introduction to stochastic partial differential equations and illustrate the characteristics of numerical schemes for this type of equation. The approximation requires a discretization in space and time and an approximation of the driving stochastic process. As an example, we consider the stochastic primitive equations and discuss specifics and problems that arise in the numerical analysis of these equations.

This is joint work with Josefin Ahlkrona and Jannik Wege.