YRM & CSE WORKSHOP PLÖN 2019

Young Researchers Meeting & Computational Science and Engineering Workshop

BOOK OF ABSTRACTS

18th to 21st March, 2019, Plön

Coordinators:

Thomas Slawig	CAU Kiel
Sabine Le Borne	TU Hamburg
Michael Hinze	Univ. Hamburg
Armin Iske	Univ. Hamburg
Jan Modersitzki	Univ. Lübeck
Malte Braack	CAU Kiel

Young Researchers Meeting

18th March, 2019

Monday YRM

14:00 **Willi Leinen**, TU Hamburg

Analysis of the discretization error in the RBF-FD method

Partial differential equations can be solved numerically by the RBF-FD method, which can be viewed as a generalization of the finite difference method to unstructured point sets. A so-called stencil is computed for each interior node which involves its nearest neighbor nodes. A radial basis function (RBF) with a given shape parameter is used for the computation of the stencil weights. The discretization error depends on the type of the point set, i.e., on the number of interior and boundary nodes and their distribution, the stencil size, the RBF and the shape parameter of the RBF. In this talk, we present an introduction to the RBF-FD method and a numerical analysis of the influence of the various parameters on the discretization error.

14:30 **Vincent Griem**, TU Hamburg

QR Decomposition of Hierarchical Matrices

Hierarchical matrices are data-sparse approximations of non-sparse matrices and allow performing most matrix operations with almost linear complexity $\mathcal{O}(n \log^{\alpha} n)$ for $1 \leq \alpha \leq 2$. There are also several algorithms to compute the QR decomposition of a hierarchical matrix with hierarchical factors Q and R, but unfortunately all are prone to numerical instability. A new algorithm based on compact WY representations and the recursive QR decomposition by Elmroth and Gustavson promises to solve this problem for a subclass of hierarchical matrices. This talk will shortly introduce hierarchical matrices and give an overview of the different QR decompositions. We will focus on the new algorithm and show a possible extension to all hierarchical matrices.

15:00 **Denis Korolev**, University of Hamburg

Reduced basis methods for parametrized linear parabolic problems

Parametrized parabolic partial differential equations occur in various complex applications, in particular, in multiphysics modelling and PDE-constrained optimisation. The multiple simulations for these problems represent a huge computational effort. Therefore, there is an increasing demand for efficient reduced models. The reduced basis techniques provide low-dimensional models for quick and robust multi-query simulations. The talk will emphasise the basics of reduced basis methods such as greedy procedure, a-posteriori error estimation, residual evaluation and parameter separability. Possible applications to PDE-constrained optimisation will be discussed.

Alessandro Cotronei, CAU Kiel **16:00**

Climate Model Optimisation by Single Precision

An ambitious project in the PALMOD climate modeling initiative is to run a complete climate simulations covering a timespan of 125.000 years. In the current state of the art, this simulation would require about 10 years on a supercomputer. It is necessary to optimise the code, in particular the most time-consuming parts like ECHAM6 and its radiation. One strategy seems to be really promising for the purpose; using “less precise” variables in the code.

Markus Pfeil, CAU Kiel **16:30**

Approximation of marine ecosystem models using artificial neural networks

he prediction of an artificial neural network can approximate the steady annual cycle of a marine ecosystem model and the computational effort of this predicition can be neglected. The computation of steady annual cycles of marine ecosystem models is important for the investigation of the carbon uptake and storage of the earth's ocean. For a three-dimensional marine ecosystem model, this computation is part of the simulation of marine biogeochemistry as well as part of optimizations of the model parameters for biogeochemical models (e.g. parameter identification are ususally done by an optimization algorithm). In this process the computation of one steady annual cycle - without using the prediction of the artificial neural network - takes up to 10000 model years and requires several hours on a high performance computing cluster. This simulations and optimizations are coupled simulations of the ocean circulation and the marine biogeochemistry. For this simulations we used an offline simulation with pre-computed ocean transport based on the transport matrix approach. Using this offline simulation we calculated 100 steady annual cycles to train an artificial neural network. We obtained by the prediction an approximation of the steady annual cycle with neglectable computational effort. However, this approximation did not conserve the mass and this approximation is consequently in need of improvement. In order to improve the approximation we adapted the prediction to conserve mass. Furthermore, we applied the predicition of an artificial neural network as initial value for the offline simulation. Thereby, we reduce the required model years of the steady annual cycle computation.

Monday YRM

17:00 **Hagen Söding**, University of Hamburg

Kernel matrices with off diagonal decay

Kernel matrices arise in the context of multi dimensional interpolation. Let $X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d$ be a set of interpolation points and $f_X = [f_1 \ldots f_n] \in \mathbb{R}^n$ a set of values. One seeks a function $s \in \mathcal{S}$ in a suitable function space $\mathcal{S}$ such that $s(x_i) = f_i$ for all x_i. Let $\mathcal{B} = \{s_1, \ldots, s_n\}$ be a basis of $\mathcal{S}$. The solution is of the interpolation problem is of the form $s(\cdot) = c_1 s_1(\cdot) + \ldots + c_n s_n(\cdot)$ with $c = [c_1 \ldots c_n]^T$ beeing the solution of the linear system

$$\begin{bmatrix} s_1(x_1) & \ldots & s_n(x_1) \\ \vdots & \ddots & \vdots \\ s_1(x_n) & \ldots & s_n(x_n) \end{bmatrix} c = f_X \quad \text{for } c \in \mathbb{R}^n$$

One often chooses radial basis functions for the interpolation, which show strong local behaviour. To approximate the interpolation matrix, one thus tries to order the data points in such a way, that points close in $\mathbb{R}^d$ are also placed close in the matrix ordering, such that the important information is gathered around the main diagonal. We present two closely related algorithms based on dimensional reduction techniques. This talk is based on joint work with Armin Iske.

17:30 **Björn Baran**, MPI Magdeburg

Large-scale Non-autonomous Differential Riccati Equations

Our motivating example is the feedback stabilization of a two-dimensional two-phase Stefan problem. After linearization and discretization, it results in a non-autonomous differential Riccati equation (DRE) with differential-algebraic structure. The Stefan problem can model solidification and melting of pure materials. This model gets its name from the purely algebraic Stefan condition which describes the coupling between the temperature of the material and its melting process. Even more differential-algebraic structure is introduced through the coupling of the Stefan problem with the Navier-Stokes equations. The two phases in the domain evolve, which causes all coefficients of the resulting DRE to be time-varying. In the literature there exist several methods to numerically solve DREs, e.g. backward differentiation formulas (BDF), Rosenbrock methods, and splitting methods. These methods are well studied for autonomous DREs. However, several difficulties arise when they are adapted to solve non-autonomous DREs, like time dependent terms that vanish only in the autonomous case and larger memory costs for the time-varying data. We present several techniques to tackle the difficulties and implement a non-autonomous BDF method.

Computational Science and Engineering Workshop

19th to 21st March, 2019

Tuesday CSE

14:00 **INVITED TALK**

Katharina Schratz, KIT Karlsruhe

Low-regularity integrators for dispersive equations

A large toolbox of numerical schemes for the nonlinear Schrödinger equation has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever "non-smooth" phenomena enter the scene such as for problems at low-regularity and high oscillations. Classical schemes fail to capture the oscillatory parts within the solution which leads to severe instabilities and loss of convergence. In this talk I present a new class of Fourier integrators for the nonlinear Schrödinger equation at low-regularity. The key idea in the construction of the new schemes is to tackle and hardwire the underlying structure of resonances into the numerical discretization. These terms are the cornerstones of theoretical analysis of the long time behaviour of differential equations and their numerical discretizations and offer the new schemes strong geometric structure at low regularity.

15:00 **Christian Kahle**, TU München

Finite element error estimates in $L^2(\Omega)$ for regularized discrete approximations to the obstacle problem

We consider the standard obstacle problem in a convex and polyhedrally bounded domain Ω with forcing $f \in L^\infty(\Omega)$, i.e. the variational inequality: Find $u \in \mathcal{K}_\Psi := \{v \in H_0^1(\Omega) \,|\, v \geq \Psi \, a.e. \text{ in } \Omega\}$ such that

$$(\nabla u, \nabla(v-u)) \geq (f, v-u) \quad \forall v \in \mathcal{K}_\Psi. \tag{VI}$$

Here $\Psi \in W^{2,\infty}(\Omega)$ is the given obstacle. Under the reasonable assumption of inactivity close to the boundary $\partial\Omega$ we derive quasi optimal error estimates for a numerical approximation of (VI) based on a regularisation approach. Namely we obtain second order convergence (up to logarithmic terms) with respect to the spatial discretization, which is assumed to be quasi-uniform. No discrete maximum principle is required. This is cooperation with Dominik Hafemeyer and Johannes Pfefferer.

Utku Kaya, Kiel University **16:00**

Local pressure corrections for incompressible flows

Since the pionnering works of Chorin and Temam [1,2], pressure correction methods have become the most popular temporal discretization techniques for the incompressible flow problems. These class of techniques consist of several substeps for each time step, which uncouples viscous diffusion and incompressiblity effects. The common approach consists of following steps:

- (i): compute a non-divergence free velocity field with the pressure from previous time step,
- (ii): compute a pressure increment from divergence error,
- (iii): project the velocity field from step (i) onto the space of divergence free vectors.

In certain applications, step (i) can be computed explicitly with time step size restrictions for stability. As a consequence, step (ii) - which is a Poisson problem - remains to be the most expensive part of the scheme. The assosicated matrix has a condition number $\sim \mathcal{O}(h^{-2})$ where h denotes a spatial mesh size. In this work we propose a domain decomposition method which approximates step (ii) without direct communication between sub-regions. Hence, the proposed method is well-suited for parallel implementation. We stress the fact that asymptotic convergence of the original method (in time) is not effected from this modification. Numerical experiments also support the theoretical results.

Marion Dziwnik, University of Hamburg **16:30**

The role of degenerate mobilities in Cahn-Hilliard models

In this talk we elucidate the role and influence of degenerate mobilities in phase field models for interface diffusion dewetting. The equation of interest is the Cahn-Hilliard equation (in two space dimensions) with a polynomial double well free energy and different order-parameter dependent, degenerate mobilities. In contrast to some results found in the literature, a detailed matched asymptotic analysis shows that the sharp interface limit is non-unique, and subtly dependents on the degeneracy of the mobility. Whilst a quadratic degenerate mobility leads to a sharp interface model where bulk diffusion is present at the same asymptotic order as surface diffusion, higher degenerate mobilities lead to a sharp interface model where bulk diffusion is sub-dominant. In particular, the corresponding numerical simulations reveal that the degeneracy has a qualitative impact on the evolution: Considering the dewetting process of a thin solid film, the evolution with bi-quadratic degenerate mobility turns out to be more effective for film pinch-off than with quadratic degenerate mobility. The results will be compared an related to other Cahn-Hilliard type models where diffusional mobilities play a decisive role.

Tuesday CSE

17:00 **Benedict Philippi**, CAU Kiel

Modification of Parareal with application to hyperbolic problems

Parallelization-in-time (PinT) methods provide an additional possibility in runtime reduction when speed-ups obtained by spatial parallelization are saturated. In climate research the concept of PinT is of particularly interest, since the models are optimized for rather low resolutions for which the benefit of spatial parallelization is limited. Among various PinT methods the Parareal algorithm offers further runtime reduction without touching the climate model routines themselves, which is a preferable property accompanied by several problem specific obstacles, especially when it comes to hyperbolic partial differential equations. This talk will address these problems and show how to modify Parareal in order to efficiently apply the algorithm, though.

Wednesday CSE

09:00 **INVITED TALK**

Peter Benner, MPI Magdeburg

Low-rank tensor methods for PDE-constrained optimization under uncertainty

We discuss optimization and control of unsteady partial differential equations (PDEs), where some coefficient of the PDE as well as the control may be uncertain. This may be due to the lack of knowledge about the exact physical parameters, like material properties describing a real-world problem ("epistemic uncertainty") or the inability to apply a computed optimal control exactly in practice. Using a stochastic Galerkin space-time discretization of the optimality system resulting from such PDE-constrained optimization problems under uncertainty leads to large-scale linear or nonlinear systems of equations in saddle point form. Nonlinearity is treated with a Picard-type iteration in which linear saddle point systems have to be solved in each iteration step. Using data compression based on separation of variables and the tensor train (TT) format, we show how these large-scale indefinite and (non)symmetric systems that typically have 10^8 to 10^{15} unknowns can be solved without the use of HPC technology. The key observation is that the unknown and the data can be well approximated in a new block TT format that reduces complexity by several orders of magnitude. As examples, we consider control and optimization problems for the linear heat equation, the unsteady Stokes and Stokes-Brinkman equations, as well as the incompressible unsteady Navier-Stokes equations. The talk surveys already published results and provides new results for the Navier-Stokes case.

Claus Goetz, University of Hamburg **10:00**

Reconstruction based DG methods: Features and Challenges

Two of the most popular families of high order schemes for hyperbolic conservation laws are reconstruction-based finite volume schemes and discontinuous Galerkin (DG) methods. The PN PM philosophy presented in Dumbser et al. (J. Comput. Phys., 227:8209–8253,2008) provides a unified framework for the treatment of both approaches. In a PN PM scheme, the solution is represented in a finite element space of piecewise polynomials of degree N (hence the PN in the name of the method) and at each time step before the time evolution is carried out, a high order reconstruction of piecewise polynomials of degree M ¿= N is computed (hence the PM). In this framework, the pure DG method can be viewed as a PN PN scheme, while the case P0 PM corresponds to the high order finite volume schemes. For N > 0 and M > N a family of hybrid schemes emerges. We study some theoretical aspects of PN PM schemes and show analytically why these methods are, in general, not L2 -diminishing. To this end, we extend the famous cell square entropy stability result of Jiang and Shu (Math. Comp. 62:531–538, 1994) for DG methods to the PN PM case and identify which part in the reconstruction step may cause the instability. With this insight we design a flux limiter that enforces a cell square entropy condition for PN PM schemes in 1D.

Michael Hinze, University of Hamburg **11:00**

Uniqueness of global solutions in VI-constrained optimization

We consider an optimal control problem subject to the elliptic obstacle problem together with its variational discretization, where we provide a condition which allows to decide whether a solution of the necessary first order conditions is a global minimum. This condition can be explicitly evaluated at the discrete level. Furthermore, we prove that if this condition holds uniformly with respect to the discretization parameter the sequence of discrete solutions converges to a global solution of the corresponding limit problem.

Ahmad Ahmad Ali, University of Hamburg **11:30**

Reduced basis method–application to elliptic control problems and variational discretization

We consider a class of parameter-dependent optimal control problems of elliptic PDEs with constraints of general type on the control variable. Applying the concept of variational discretization(Hinze 2005), together with techniques from the Reduced basis method, we construct a reduced basis surrogate model for the control problem. We establish estimators for the greedy sampling procedure which only involve the residuals of the state and the adjoint equation, but not of the gradient equation of the optimality system. The estimators are sharp up to a constant, i.e. they are equivalent to the approximation erros in control, state, and adjoint state. Numerical experiments show the performance of our approach.

Wednesday CSE

14:00 **Armin Iske**, University of Hamburg

Model-based design of kernel approximation methods for data analysis

We show how to design kernel-based approximation schemes in situations where standard kernel methods are not suitable or even doomed to fail. To this end, we first discuss the characterization and construction of non-standard kernels for data analysis on the basis of specific model assumptions. This leads us to a larger class of flexible kernel-based approximation methods, relying on weighted kernels that are symmetric but not radially symmetric. Further in our discussion, we then turn to the design of kernel-based regularization methods, as they are relevant in applications of machine learning. We address numerical aspects and, moreover, we provide numerical examples for further illustration.

14:30 **Robin Ahrens**, TU Hamburg

Estimation of aggregation kernels from time-sparse measurements

The field of particle technology models processes such as growth, aggregation and breakage using population balance equations which involve integro partial differential equations. In this talk we focus on the aggregation process in which the integral kernel models the rate at which particles agglomerate. This kernel is typically designed based upon physical properties of the involved particles and their environment. Here, we address the inverse problem which consists of reconstructing the kernel given the data measured in experiments. We introduce two different approaches and illustrate their performance through numerical experiments.

15:00 **Thomas Slawig**, CAU Kiel

Kernel Density Estimates in Marine Ecosystem Modeling and Parameter Optimization

We show examples of the application of non-parametric statistics used for model intercomparison and parameter estimation. Our research field is marine ecosystem modeling as one important part of Earth system models. These models describe the marine part of the global carbon cycle and are crucial for climate predictions. Many of the inherent parameters are only estimated and are usually determined via minimization of a model-data misfit function. On one hand, the optimization process of the 3-D and coupled models is a challenging task. On the other hand, the choice of an appropriate cost or misfit function also influences the results. We show methods of kernel density estimation via Gaussian kernels in recent applications of the "PalMod" project. Aim of this German climate modeling initiative is to compute a complete glacial cycle with comprehensive Earth system models. We also discuss our plans for more general diffusion kernels. This is joint work with Markus Schartau and Christopher Somes from the Helmholtz Centre for Marine Research Kiel (GEOMAR).

Sabine Le Borne, TU Hamburg **16:00**

Direct solvers for RBF interpolation problems

Scattered data approximation deals with the problem of producing a function s that in some sense represents some given (typically scattered) data and allows to make predictions at other times/locations/parameter settings. Applications are quite diverse: Surface reconstruction, image compression, numerical solution of PDEs (with their diverse applications), to name just a few. In a scattered data interpolation problem, the interpolant is typically a linear combination of some radial basis functions (RBF). The coefficient vector $c \in R^N$ of the interpolant may be computed as the solution of a linear system $Bc = y$ which results from enforcing the interpolation conditions for the given scattered data. While properties of the matrix B obviously depend on the choice of basis functions, several of the most commonly used approaches yield highly ill-conditioned, dense matrices B, resulting in a challenge to solve the linear system $Bc = y$, and hence to solve the scattered data interpolation problem. This talk deals with these challenges and some possible strategies for the solution of this system $Bc = y$. In particular, we study the application of techniques from the $\mathcal{H}$-matrix framework both for the approximation of the system matrix B itself as well as for the construction of solvers. $\mathcal{H}$-matrices provide a data-sparse matrix format that permits storage and matrix arithmetic in complexity $\mathcal{O}(N \log^\alpha N)$ for moderate α. It turns out that several typical sets of basis functions from the (scattered data) literature lead to matrices B that fit into this framework, yielding a cost-effective approximation scheme to be illustrated in this talk.

Heiko Kröner, University of Hamburg **16:30**

Analysis and an Interior Point Approach for TV Image Reconstruction Problems on Smooth Surfaces

Lai and Chan [Computer Vis. Image Underst., 115 (2011), pp. 1647–1661] introduced an analogue of the total variation image reconstruction approach of Rudin, Osher, and Fatemi [Phys. D, 60 (1992), pp. 259–268] for images on smooth surfaces. The problem is defined in terms of quantities intrinsic to the surface and is therefore independent of the parametrization. In this paper, a rigorous analytical framework is developed for this model and its Fenchel predual. It is shown that the predual of the total variation problem is a quadratic optimization problem for the predual vector field $q \in H(\mathrm{div}; S)$ with pointwise inequality constraints on the surface. As in the flat case, q serves as an edge detector. A function space interior-point method is proposed for the predual problem, which is discretized by conforming Raviart–Thomas finite elements on a triangulation of the surface. Well-posedness of the barrier problems is established. Numerical examples including denoising and inpainting problems with both gray-scale and color images on scanned three-dimensional geometries of considerable complexity are presented.

Thursday CSE

09:00 **INVITED TALK**

Luise Blank, University Regensburg

ptimization with convex constraints and an application in topology optimization

This talk focuses on projection type methods for convexly constrained optimization problems. We shortly introduce well known projection methods using the gradient in finite dimensions and summarize known results. Varying the underlying scalar product allows to include second order information to speed up the method. E.g. the projection of the Newton direction leads to a quadratic order of convergence. The method can also be interpreted as solving a sequence of optimization problems where the cost function is quadratically approximated. Results in function spaces are important to obtain methods with iteration numbers independent ot the discretization level. They also indicate which underlying metric shall be used for the projection. E.g. pde constraint problems provide often only differentiability of the cost functional in the L^∞ metric. While the generalization to Hilbert spaces is straight forward the extension to Banach spaces is more involved due to the missing scalar product. We present a global convergence result for the variable metric projection type (VMPT-)method, which allows application to nonreflexive Banach spaces and expand the possible choices of the metric. Moreover, we give examples which fulfill the requirements on the spaces and the variable metric. As an application we consider a structural topology optimization problem. The model is based on a diffuse interface ansatz using phase field variables. The necessary regularization of the cost functional with the perimeter is substituted by the Ginzburg-Landau energy. We obtain a minimization problem with pde constraints and simplex constraints for the controls. The elimination of the state using the nonlinear control-to-state operator yields a convexly constrained optimization problem, where we can apply the VMPT-algorithm in $L^\infty \cap H^1$. In the numerical results one can clearly see that choosing an appropriate inner product, namely H^1, leads –in contrast to L^2– to mesh independency of the iteration numbers. Including additionally second order information speeds up the method drastically.

10:00 **Niklas Kühl**, TU Hamburg

Optimization with convex constraints and an application in topology optimization

This presentation discusses an extension of the classical Volume-of-Fluid (VoF) method with a diffusive term derived from a Cahn-Hilliard (CH) approach. Aiming at efficient simulations of quasi-static two-phase flows, we can outperform a compressive-scheme based VoF-procedure by almost an order of magnitude computing effort. Formally, the CH Navier-Stokes system refers to a concentration transport equation which contains a number of additional, unfavorable terms, that are for example associated to 4th-order derivatives or severe non-linearities. Moreover, the VoF-related velocity field is no longer divergence-free.

[Continued on next page]

Niklas Kühl, TU Hamburg **10:00**

However, if surface tension is insignificant, this equation can be converted into a classical convection-diffusion equation, which inherently provides a sharp phase transition without the use of compressive, downwind-biased approximations of convective kinematics. Introducing an alternative, differentiable equation of state, that is motivated by an analytical solution to two-phase shear-flows, the procedure is strongly regularized. A remaining free mobility constant of the concentration equation is divided into a physical and an artificial (numerical) component. The latter is assigned to computed values that eliminate the numerical diffusion originating from approximation of the convective kinematics. Using classical upwind formulae, the usual time-step restriction vanishes. Verification and validation are performed for a variety of 1D and 2D test cases, including analytical solutions. Applications address 3D simulations of a fully turbulent flow around a container ship at operating points of practical relevance. Examples included demonstrate the robustness and the greatly improved efficiency of the present method.

Carmen Gräßle, University of Hamburg **11:00**

POD model order reduction with space-adapted snapshots for incompressible flows

We consider model order reduction for unsteady incompressible Navier-Stokes problems. A reduction of computational complexity is achieved by a Galerkin projection of the solution of a high-dimensional problem onto a low-dimensional subspace. We focus on subspaces generated by a proper orthogonal decomposition (POD) of space-adapted finite element snapshots. In previous works, we have investigated adaptive POD-Galerkin modeling for elliptic and parabolic problems. Incompressible flows impose additional challenges regarding the stability of the resulting reduced-order models and regarding the implementation of inhomogeneous initial and boundary conditions. We propose two approaches to computing reduced spaces which result in stable POD-Galerkin models. The first approach employs a projection of the adapted velocity snapshots onto a space of functions which are weakly divergence-free with respect to a pressure reference space. The resulting reduced-order model is a system of ordinary differential equations for the velocity POD coefficients. The second approach is based on separate PODs of the adapted velocity and pressure snapshots. Here, the velocity POD basis is enriched by supremizer functions computed on a reference velocity space. The stability of the velocity-pressure pair of reduced spaces is linked to the inf-sup constant of the reference discretization. We analyze the complexity of the proposed reduced-order models, present numerical results for a benchmark problem, and compare our methods in terms of accuracy per computational cost.