Young Researchers Meeting
&
Recent trends and future developments in Computational Science and Engineering

(CSE Plön 2020)

Book of abstracts

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

23. - 26.03.2020

Contents

Young Researchers Meeting (YRM) - Mon, 23.03.2020

Program

Session YRM I: 13:30 - 15:30

13:30 - 14:00: Sofiya Onyshkevych (UHH)

Shape Optimization in Navier-Stokes Flow

The problem of finding optimal shape design is of great practical importance in many engineering applications such as ship components, aircraft wings, and turbines. In the present work, we consider the shape optimization problem of a solid body in an incompressible stationary Navier-Stokes flow. We strive to find the optimal shape of the obstacle immersed in the fluid flow with respect to some measurement of interest, e.g. drag. The shape optimization problem is formulated on a fixed reference domain via the method of mappings. Further, following the optimize-then-discretize approach, the Lagrangian-based optimality conditions are derived, whereas the actual optimization is conducted in a one-shot manner. Moreover, we investigate extension operators to achieve high mesh quality and guarantee suitable shape spaces. Finally, we present some numerical results obtained using the FEniCS Project software.

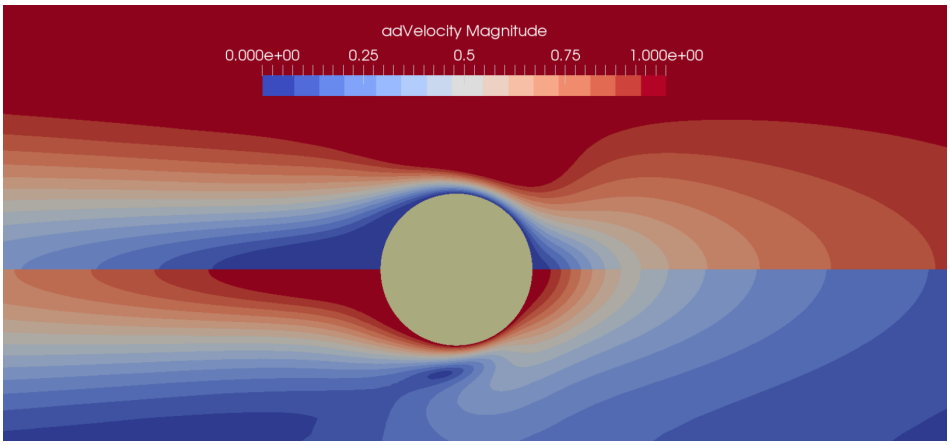
14:00 - 14:30: Peter M. Müller (TUHH)

Decoupling of Control and Force Objective in Adjoint-Based Fluid Dynamic Shape Optimization

joint work with: Niklas Kühl (TUHH), Arthur Stück (German Aerospace Center (DLR)), Michael Hinze (Uni Koblenz), Thomas Rung (TUHH)

We discuss exterior and classical interior alternatives for evaluating fluid flow induced forces on bodies. The discussion aims at a reduction of the total shape derivative, achieved through a decoupling of control and objective in the exterior approach. In this case, geometric as well as convective contributions to the shape derivative vanish. Convective contributions depend on primal physics and may disappear, which is not the case for geometric components. The latter can be interpreted as curvatures immanent to industrial applications. The remaining local derivative of the objective functional can be determined efficiently with an adjoint system, that differs to the classical approach in its boundary conditions only and resembles an ALE strategy 1. A

two-dimensional flow exposed to gravity illustrates the features of the exterior approach, whereby carefully derived derivatives from a second order Finite-Difference study were used to validate the results.



Adjoint velocity magnitude in the direct cylinder vicinity at $Re_D = 20$ and $Fn_D = 0.25$

14:30 - 15:00: Markus Pfeil (CAU Kiel)

Surrogate-based optimization using an artificial neural network

The prediction of an artificial neural network reduced the computational costs of a parameter identification for a three-dimensional marine ecosystem model using a surrogate-based optimization. Marine ecosystem models are important for the investigation and prediction of the climate change especially of the carbon uptake and storage of the earth's ocean. Determining the parameter of a marine ecosystem model is a challenging task in ocean modeling. In particular, the optimization runs are computationally expensive because a single simulation of a marine ecosystem model - without using the prediction of an artificial neural network - takes several thousand model years and requires several hours on a high performance computing cluster. These simulations

are fully coupled simulations of the ocean circulation and the marine biogeochemistry. We used, however, an offline simulation with pre-computed ocean transport based on the transport matrix approach.

The surrogate-based optimization is a method to accelerate the optimization process. For this purpose, the original and computationally expensive (high-fidelity) model is replaced by the so-called surrogate, which is the result of a less accurate but computationally cheaper (low-fidelity) model and a multiplicative correction operator. We used the prediction of an artificial neural network as low-fidelity model.

We trained an artificial neural network applying the sparse evolutionary training algorithm in combination with a genetic algorithm to find an appropriate network topology of the neural network. We obtained an approximation of the simulation of the entire marine ecosystem model with neglectable computational effort by the prediction of the artificial neural network. Thereby, we shortened the computational time of the parameter identification for a marine ecosystem model using the surrogate-based optimization.

15:00 - 15:30: Maria-Theresia Verwega (GEOMAR / CAU Kiel)

Finite element based implementation of the
diffusion kernel density estimator
enables analysis of unknown data sets

Estimating the distribution of an unknown data set is one major task of statistics. This is often transferred to instead approximating the probability density function (PDF). The PDF is, if it exists, is the derivative of the distribution. A well-known measure for this task is the non-parametric approach of kernel density estimation (KDE).

To the best of our knowledge, all available implementations of KDE suffer from shortcomings when applied to differing kinds of data sets. The most common KDE is the Gaussian KDE. This works fast, but is known to be inconsistent at the boundaries of restricted intervals and tends to overs-mooth multimodal data. A different approach is the diffusion KDE, which is superior to the Gaussian in terms of structure resolution. But its implementations become slower up to unapplicable with increasing data set size.

We developed a new implementation of the diffusion KDE, which we found to work fast and reliable for data sets of only few up to 100.000 data points with boundary close values and multiple modes. Our implementation is based on a finite element (FEM) discretization and realized in the FEM software framework FEniCS.

We tested our implementation in direct comparison to the traditional Gaussian on artificial and real marine biogeochemical data. We conclude our implementation being well suited for analyses of unknown data sets with varying sizes, distributions and number of modes.

Session YRM II: 16:00 - 18:00

16:30 - 17:00: Heena Patel (UHH)

Multiscale methods application to Canopies in Earth System

The urban canopies consist of buildings or trees that are aligned along a street in the horizontal direction. These canopies in cities and forests modulate the local climate considerably in a complex way. Climate models strive to represent such subgrid features that actually play significant impact on Earth System components that is Atmosphere, Land and Ocean. Multiscale finite element methods have been applied to various porous media applications. In order to study the effect of various parameters like pollutant, velocity of wind and temperature on the atmospheric boundary layer, a semi-Lagrangian multiscale framework for the advection-diffusion equation is studied. It is composed of two parts: an offline phase that precomputes the basis functions and an online phase that uses these basis functions to compute the coarse solution. The core idea of MsFEM is that the basis functions are constructed such that subgrid-scale information is imprinted on them. The overhead of precomputing the basis functions in each coarse block can further be reduced by parallelization. The online phase is approximately as fast as a low resolution standard FEM but still reveals fine scale features of a highly resolved solution and is therefore accurate. This approach is studied in order to modulate the effect of different scales present in climate simulation models with canopy effect on atmospheric boundary layer. Different cases are studied with changes in Pélect number and Courant number. The computational method will be compared

with transport in a wind tunnel experiment carried out in University of Hamburg. The solutions obtained from these methods are then validated with high resolution data available from urban simulation in order to verify the accuracy to represent subgrid phenomena in climate models.

The high resolution urban simulation will be conducted with Computational Fluid Dynamics (CFD) software with fully developed atmosphere boundary layer as inlet condition. A three dimensional domain is considered where canopies are created as blocks and forests as Leaf Area Density (LAD) for forest profiles in OpenFoam 6 software. The simulation will be configured for different scenarios with velocity and temperature by Large Eddy Simulation (LES). Further, a source that emits gas will be considered in order to see how canopies effects the atmosphere boundary layer in presence of a pollutant gas.

17:00 - 17:30: Willi Leinen (TUHH)

Analysis of the discretization error in the RBF-FD method

Partial differential equations can be solved numerically by the radial basis function-generated finite difference (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. We focus on Poisson's equation and on the convection-diffusion equation in three-dimensions.

17:00 - 17:30: Kristoff Albrecht (TUHH)

Greedy methods in kernel-based learning

Machine learning requires high-performance algorithms from multivariate data analysis, in particular for reliable predictions and fast evaluations. To this end, meshfree kernels are powerful tools from approximation, especially for critical (i.e., very large, scattered and high-dimensional) data, where multilevel approximation schemes are combined with greedy algorithms for the construction of suitable data hierarchies.

This talk discusses efficient greedy methods, which are well-adapted to the particular requirements of kernel approximation schemes. Moreover, we explain how to maintain orthonormal kernel systems, along with the construction of the data hierarchies. This will result in numerically stable kernel reconstruction methods, whose further advantages will be demonstrated by numerical simulations

17:30 - 18:00: Roland Haase (Uni Lübeck)

Explicitly constrained robust PCA for groupwise image registration

Rank minimization is a widely-used approach to measure the similarity between groups of multiple images in variational image registration. Robust Principal component analysis (RPCA) is often employed to ensure robustness against distortions such as occlusions or local changes in image intensity (e.g., in DCE-RMI). In this talk, we will discuss some pitfalls of the classical Principal Component Pursuit (PCP) from (Candes et al., 2011) and propose a more suitable replacement in the context of measuring groupwise image dissimilarity. Like PCP, the proposed measure, which we term δ-RPCA, is given by the energy of an optimal data decomposition into low-rank and sparse components, in which low-rankness is modeled through explicit constraints instead of soft penalties. Given its definition, this new approach especially lends itself to image sequences that involve objects with recurring changes in appearance as well as sparsely distributed distortions.

We combine the $\delta - PRCA$ masure with total variation regularization into a fully deformable non-parametric registration scheme. Special attention is paid to the question of ensuring unique solutions that generally arises in groupwise image registration. Numerical results of the motion correction capabilities of our model are shown and analyzed both in terms of the registration accuracy and the generated data decomposition.

Computational Science & Engineering (CSE) - Tue, 24.03.2020

Program

Invited Lecture

13:30 - 14:30: Euan Spence (University of Bath)

Resolution of a long-standing open question in the numerical analysis of boundary integral equations for Laplace's equation

Boundary integral equations were introduced in the 19th century to study Laplace's equation. Today they are used extensively in applied maths and industry to compute approximations of the solutions to Laplace's equation (and other PDEs), with many numerical schemes based on the Galerkin method. Perhaps surprisingly, however, it has not yet been proved whether or not the Galerkin method converges when applied to the standard second-kind boundary integral equations for Laplace's equation on general Lipschitz domains, or even general $3d$ Lipschitz polyhedra.

In this talk, I will describe recent results obtained with Simon Chandler-Wilde (University of Reading) that settle this question.

Session CSE I: 14:30 - 15:30

14:30 - 15:00 Marion Dziwnik (UHH)

Diffusion vs. surface diffusion: dynamics and stability of self-similar pinchoff

This talk elucidates the differences between (bulk-)diffusion and surface diffusion concerning the dynamics and stability of self-similar Pinch-off. Both models conserve the volume enclosed inside some surface while minimizing its surface area. We review the axisymmetric equilibria: the cylinder, the sphere, and the Delaunay unduloid. In both models, the sphere is stable, while the cylinder is long-wave unstable and a subcritical bifurcation from the cylinder produces a continuous family of unduloid solutions. Even though both model feature similar characteristic stability properties, numerical simulations show that the surface diffusion model is more likely to show pinch-off than the (bulk-)diffusion model. We explain this phenomenon with computations that suggest that perturbed

unduloids rather relax to the cylinder in the (bulk-) diffusion case while tending towards finite-time pinchoff in the surface diffusion case.

15:00 - 15:30 Hannes von Allwörden (UHH)

Classification of stop-and-go waves in microscopic traffic flow models

joint work with: Ingenuin Gasser (UHH)

From a driver's perspective, stop-and-go waves are an undesirable yet common feature of real-life traffic. Their emergence has also been demonstrated in classical circular road experiments under controlled conditions. In this setting they can be mathematically understood as headway-periodic solutions emerging from Hopf bifurcations of quasi-stationary solutions in a finite-dimensional system of ordinary differential equations. These can be numerically traced through parameter space by continuation algorithms. We consider the behaviour of such solutions on the transition to an open road with infinitely many vehicles on it and discuss approaches to parametrise and classify them.

Session CSE II: 16:00 - 17:30

16:00 - 16:30: Thi Bich Tram Do (UHH)

Discrete regularization for parameter identification problems

This work is concerned with inverse problems where a distributed parameter is known a priori to only take on values from a given discrete set. This property can be promoted in Tikhonov regularization with the aid of a suitable convex but nondifferentiable regularization term. Using the specific properties of the regularization term, it can be shown that convergence actually holds pointwise. Furthermore, the resulting Tikhonov functional can be minimized efficiently using a semi-smooth Newton method. Convergence rates of the method is obtained under condition on measure of active sets. Additionally, total variation is added to promote regularity on the boundary of the reconstructions.

16:30 - 17:00: Christiane Schmidt (UHH)

Dynamic concentration reconstruction for magnetic particle imaging using splines

Magnetic particle imaging (MPI) is a new imaging technique using the nonlinear response of superparamagnetic iron oxide nanoparticles (SPION) to changing magnetic field strengths. Injecting a patient with a SPION- tracer an MPI scanner uses electromagnetism to locate the tracer concentration. The tracer circulates or accumulates in certain regions of the patient's body until it is dissipated. MPI enables noninvasive examinations of physiological processes without ionizing radiation.

Reconstruction of time series of the dynamic behavior of the tracer concentration is therefore highly relevant from a diagnostic point of view. Dynamic inverse problems have not yet been studied in depth. MPI images often consist of several subsequently scanned patches. Therefore, there is a time gap in between successive frames which impedes using the similarity of successive frames for regularization in the reconstruction process. One approach which also takes this into account will be presented in this talk.

17:00 - 17:30: Matthias Beckmann (UHH)

On a new non-linear inverse problem involving the Radon transform

joint work with: Ayush Bhandari (Imperial Col. London) and Felix Krahmer (TUM)

High dynamic range tomography is one of the current research topics in the field of computerized tomography and addresses how to deal with information loss due to sensor saturation or clipping effects. This occurs whenever the dynamic range of the measured X-ray projections exceeds the sensor's recordable threshold. Existing methods typically rely on the fusion of multiple exposures. In contrast, we propose a one-shot approach based on a non-linear inverse problem involving a generalization of the conventional Radon transform. We take a first step towards invertibility of the introduced operator and propose a sequential recovery algorithm.

17:30 - 18:00: Sara Krause-Solberg (TUHH)

1-*bit compressed sensing on manifolds*

Compressed Sensing deals with reconstructing some unknown vector from few linear measurements in high dimension by additionally assuming sparsity, i.e. many entries are zero. Recent results guaranteed recovery even when just signs of the measurements are available (one-bit CS). A natural generalization of classical CS replaces sparse vectors by vectors lying on manifolds having low intrinsic dimension. In this talk I introduce the one-bit problem for data lying on manifolds and propose numerical and theoretical results.

Computational Science & Engineering (CSE) - Wed, 25.03.2020

Program

Invited Lecture

09:30 - 10:30: Christian Wieners (KIT Karlsruhe)

Space-time discontinuous Galerkin methods for linear hyperbolic systems

joint work with: W. Dörfler, J. Ernesti, S. Findeisen, and D. Ziegler

We consider variational space-time discretizations of linear first-order hyperbolic systems. Based on the theory for symmetric Friedrichs systems we establish an analytic framework and we prove inf-sup stability of the continuous variational setting.

Discrete inf-sup stability is obtained for a space-time method with discontinuous Galerkin elements with upwind flux in space and weakly continuous Galerkin elements in time. The discretization is adaptive with independent choice of polynomial degrees p in time and q in space for every space-time cell. The discretization is fully implicit, and the overall linear problem is solved with a parallel Krylov method using a multigrid preconditioner based on a subspace hierarchy. The adaptivity is controlled by a dual weighted residual error estimator with respect to a given linear error functional.

The method is evaluated for a benchmark configuration in geophysics, the full waveform inversion to identify the subsurface material distribution by seismograms. Here we consider p-adaptive approximations of the forward problem based on a dual-primal error estimator with respect to a goal functional corresponding to the seismic measurements.

[1]W. Dörfler, S. Findeisen, and Wieners, C.: *Space-time discontinuous Galerkin discretizations for linear first-order hyperbolic evolution systems*, Comput. Methods Appl. Math. 16(3):409-428, 2016

[2] W. Dörfler, S. Findeisen, C. Wieners, and D. Ziegler: *Parallel adaptive discontinuous Galerkin discretizations in space and time for linear elastic and acoustic waves*, In: Space-Time Methods. Applications to Partial Differential Equations, U. Langer and O. Steinbach, editors, volume 25 of Radon Series on Computational and Applied Mathematics, 61–88, 2019.

[3] J. Ernesti and C. Wieners: *Space-time discontinuous Petrov-Galerkin methods for linear wave equations in heterogeneous media,* Computational Methods in Applied Mathematics 19(3), 465–481, 2019

[4] S. Findeisen: *Parallel and Adaptive Space-Time Method for Maxwell's Equations*, PhD Thesis Karlsruhe 2016

[5] J. Ernesti: *Space-Time Methods for Acoustic Waves and Applications to Full Waveform Inversion*, PhD Thesis Karlsruhe 2017

[6] D. Ziegler: *A parallel and adaptive space-time discontinuous Galerkin method for visco-elastic and visco-acoustic waves*, PhD Thesis Karlsruhe 2019

Session CSE III: 11:00 - 12:30

11:00 - 11:30: Claus Goetz (UHH)

Understanding GRP solvers

The generalized Riemann problem (GRP) is the Cauchy problem for a hyperbolic conservation law with piecewise smooth data that includes a jump-discontinuity. This problem naturally occurs in high-order numerical schemes: In a finite volume scheme with a reconstruction step, or in a discontinuous Galerkin finite element method, the solution of the PDE is represented at each time-step by a piecewise smooth function with possible jumps at the cell interfaces. We are mainly interested in solving the GRP as a building block for high-order numerical schemes.

In general, no exact solutions of the GRP for nonlinear systems are available. Approximate GRP solvers typically employ one of the following strategies: (1) "Instantaneous interaction", which roughly speaking leads to a Taylor approximation of the solution; or (2) "Evolution in the small", which means evolving the solution locally in each cell and computing numerical fluxes from the evolved data without resolving the full wave-pattern of the GRP. Recently, approach (2) gained in popularity, because it is a lot easier to code and can be adapted to handle stiff source terms more easily. However, a systematic comparison of the two approaches and

a rigorous analysis of its theoretical properties seem to be missing in the literature. Our aim is to contribute a first step towards closing this gap.

In this talk we give a short introduction to the theory of both classical and generalized Riemann problems, see different GRP solver in action, and take a closer look at what evolution in the small solvers are actually trying to compute from an analytical perspective.

11:30 - 12:00: Leon Schramm (CAU Kiel)

ROW Methods and W-Methods for the Incompressible Navier-Stokes Equations

It is well-known that the temporal discretization of PDEs such as the incompressible NavierStokes equations (NS) requires highly stable, and thus, implicit schemes in order to avoid impractically small time steps. In many standard schemes, such as implicit Runge-Kutta methods (RKM), the nonlinearity in NS then leads to nonlinear systems, the solution of which is usually numerically expensive.

ROW Methods and W-Methods aim to modify RKM, so that the implicitness is reduced as much as possible, while sufficient stability is maintained. This is achieved by linearizing the equation and then handling the linear term implicitly and the nonlinear error explicitly. In ROW methods the exact Frechet derivative at the last numerical solution is used for linearization, while in Wmethods that derivative might even be approximated.

Numerical experiments with ROW methods applied to NS have been conducted and described by many authors (see for example [1, 2, 3]). On the other hand, W-methods with approximative derivatives of the nonlinearity in NS have rarely been studied in numerical tests. We present promising experimental results with several W-methods and compare the performance of those methods with that of established ROW methods and the hugely popular Crank-Nicolson method.

[1] V. John and J. Rang: *Adaptive time step control for the incompressible Navier–Stokes equations*, Comput. Method. Appl. M., 199(9-12): 514 –524, 2010

[2] J. Rang: *Improved traditional Rosenbrock–Wanner methods for stiff ODEs and DAEs*, J. Comput. Appl. Math., 286:128 – 144, 2015

[3] I. Teleaga and J. Lang: *Higher-Order Linearly Implicit One-Step Methods for Three Dimensional Incompressible Navier-Stokes Equations*, Studia Babes-Bolyai Matematica, 53(1):109–121, 2008

12:00 - 12:30: Jörn Behrens (UHH)

Efficiency metrics for adaptive mesh refinement algorithms

joint work with:
Nicole Beisiegel (UC Dublin), Cristobal Castro (Universidad de Tarapacá)

Solving practical PDE-based applications comprising multiple spatial scales often requires the utilization of adaptive mesh refinement (AMR) methods. These methods impose a substantial overhead on computational performance and their efficiency therefore needs to be assessed and monitored. This presentation will give a short introduction to a rather generic description of AMR methods, followed by descriptions of a number of different efficiency measures for different aspects of AMR. While this is a rather applied topic with relatively straight forward approaches to quantify efficiency of AMR, we hope that the systematic documentation of such metrics may help to make different schemes more comparable and assess the benefit of AMR to actual situations.

Session CSE IV: 13:30 - 15:30

13:30 - 14:00 Benedict Philippi (CAU Kiel)

In-time parallelization of hyperbolic problems

Among the various Parallel-in-Time (PinT) algorithms that provide further speedup when spatial parallelization methods have reached their limit, the common problem states a feasible solution to cope with non-linear hyperbolic (partial) differential equations. While some satisfactory achievements in linear inhomogeneous problems could be obtained, the search for an iteration procedure to parallelize non-linear problems goes on. This talk concerns the Parareal algorithm, which is an approximation to the Newton iteration for a system of general nonlinear differential equations. Modifications of the iteration procedure allow for linear inhomogeneous inital value problems while also suffering from the bad convergence, typical to PinT algorithms. Both issues and the progress so far are presented during this talk.

14:00 - 14:30 Daniel Ruprecht (TUHH)

Some recent developments in the field of parallel-in-time integration

The fundamental change of high-performance computing systems towards massive parallelism brings with it interesting and important challenges for developers of numerical algorithms. Where previously advances in algorithms and hardware contributed to simulation performance independently, new parallel algorithms are now required to unlock the computing power of parallel systems and to translate it into performance.

Many models in physical sciences and engineering come in the form of differential equations. Traditionally, efforts to parallelise their numerical solution have focussed on the three spatial coordinates, while integrating time with sequential time stepping schemes like multistep or Runge-Kutta methods. This leaves the time dimension as a bottleneck and results in both weak and strong scaling traps, limiting performance.

Although ideas to introduce concurrency in the time direction go back to 1964 [4], the field of parallel-in-time integration methods only recently became an active area of research, driven by the algorithmic challenges posed by future Exascale systems [2]. I will present two popular algorithms, Parareal [3] and PFASST [1] and show some examples how they can improve performance in massively parallel simulations. Also, I will highlight some of the challenges, in particular with respect to hyperbolic equations, and shed some light on the underlying mathematical issues [5].

[1] M. Emmett and M. L. Minion: *Toward an Efficient Parallel in Time Method for Partial Differential Equations*, Communications in Applied Mathematics and Computational Science, 7:105–132, 2012

[2] M. J. Gander: *50 years of Time Parallel Time Integration*, In Multiple Shooting and Time Domain Decomposition, Springer, 2015.

[3] J.-L. Lions, Y, Maday, and G. Turinici: *A "parareal" in time discretization of PDE's*, Comptes Rendus de l'Academie des Sciences - Series I - Mathematics 332: 661–668, 2001

[4] J. Nievergelt, *Parallel methods for integrating ordinary differential equations*, Commun. ACM, 7:731–733, 1964

[5] D. Ruprecht: *Wave propagation characteristics of parareal*, Computing and Visualization in Science, 19:1–17, 2018

14:30 - 15:00 Sebastian Götschel (TUHH)

Parallelization in time for optimal control and inverse problems

joint work with Michael Minion (Lawrence Berkeley National Lab)

Large-scale optimization problems governed by time-dependent partial differential equations (PDEs) occur in a multitude of applications, for example in inverse problems for non-destructive testing of materials and structures, or in optimal control problems related to individualized medicine. Algorithms for the numerical solution of such PDE-constrained

optimization problems are computationally extremely demanding, as they require multiple PDE solves during the iterative optimization process. With today's modern computers, the time-to-solution can be decreased through massive parallelization, which is traditionally done in the spatial dimensions. In addition, time-parallel methods have received increasing interest in recent years to overcome scaling limits. Iterative multilevel schemes such as PFASST (Parallel Full Approximation Scheme in Space and Time) are currently state of the art and can achieve significant parallel efficiency.

In this talk, we investigate approaches to use PFASST for the solution of optimal control problems and inverse problems. Besides enabling time parallelism, the iterative nature of the temporal integrators within PFASST provides additional flexibility for reducing the cost of solving nonlinear equations, re-using previous solutions in the optimization loop, and adapting the accuracy of state and adjoint solves to the optimization progress. We discuss benefits and difficulties, and present numerical examples.

15:00 - 15:30 Robin Ahrens (TUHH)

Efficient numerical treatment of aggregation integrals in multivariate population balance equations

We address the numerical computation of aggregation integrals that arise in population balance equations, a technique commonly used in particle technology. We focus on the multivariate case of pure aggregation where a particle is described by several properties and particles do not experience other phenomena like growth or breakage. The evolution of a population density distribution $f(\mathbf{v}; t)$ over time is modeled by an integro-differential equation that we solve numerically. These integrals feature a kernel $\kappa(\mathbf{u}; v)$ describing the rate at which particles with properties $\mathbf{u}$ and $\mathbf{v}$ combine to form a new larger particle with properties $\mathbf{u} + \mathbf{v}$.

For this we discretize the property space on a uniform tensor grid with N cells to turn the integrals into summations. A straight forward evaluation of these summations is of complexity $\mathcal{O}(N^2)$ and dominates the computational time during numerical simulations.

We discuss an alternate algorithm to evaluate this right hand side that is based on the separable representation (or approximation) of the aggregationkernel. This allows us to compute the result by a series of fast Fourier transformations reducing the quadratic complexity to a nearly optimal complexity of $\mathcal{O}(kN \log N)$, where k is the rank of the separation. We also present a projection to preserve physical invariants of the particle process initially lost in the discretization. We show the merits of this approach by comparing it with existing methods via numerical simulations. We additionally use the tensor-train decomposition to overcome the curse of dimensionality and reduce the storage and computational complexity even further. We are able to perform numerical simulations that otherwise exceed capabilities of supercomputers on an office-desktop computer by using this low-rank structure to approximate the density distribution. We further propose an improvement of the truncation-algorithm in order to speed up this essential computational step. We illustrate the usability of this format by extensive numerical simulations.

Session CSE V: 16:00 - 17:30

17:30 - 18:00 Sabine Le Borne (TUHH)

Mathematician meets Physicist: High performance simulations of next generation light sources

16:30 - 17:00 Vincent Griem (TUHH)

A New Approach to the 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. This talk will shortly introduce hierarchical matrices and the idea of an optimal structure of the hierarchical matrix product. We will then derive a new approach to find the QR decomposition of a hierarchical matrix based on compact WY representations and the recursive QR decomposition by Elmroth and Gustavson. Finally we provide some numerical examples.

17:00 - 17:30: Niklas Wagner (UHH)

Constructing Laplacian matrices for image compression by adaptive thinning

Adaptive Thinning (AT) is a powerful method for image compression, as introduced in [1]. The method AT regards an image as a bivariate target function, which is approximated by a linear spline over an anisotropic Delaunay triangulation. For further development, we improve the image quality on specifically selected triangles by encoding textures separately. This requires a technique which allows us to work with irregular data domains. To this end, we apply signal processing on graphs, which merges

algebraic and spectral graph theoretic concepts with computational harmonic analysis. We interpret the given data as a graph signal on a graph given over each triangle and apply the graph Fourier transform. In the graph spectral domain we are then able to apply filtering methods on the data. To achieve an efficient compression, special care should be taken when selecting each graph, so that it adapts to the given data.

[1] L. Demaret, N. Dyn, and A. Iske: *Image Compression by Linear Splines over Adaptive Triangulations*, Signal Processing 86(7):1604 –1616, 2016

Computational Science & Engineering (CSE) - Thu, 26.03.2020

Program

Invited Lecture

09:30 - 10:30 Kathrin Padberg-Gehle (Leuphana Uni Lüneburg)

Identification and characterization of coherent behavior in flows

The motion of tracers in fluids flows is crucially influenced by coherent structures. Due to their strong impact on global transport and mixing processes the characterization of these Lagrangian objects is a topic of intense current research. From a probabilistic point of view, coherent sets are regular regions in the physical domain of the flow that move about with minimal dispersion.

Coherent sets can be efficiently identified via Perron-Frobenius operators (or transfer operators). These linear Markov operators can be approximated within a set-oriented numerical framework. Subdominant singular values/vectors of the resulting stochastic matrices are then used to determine and characterize the structures of interest.

While transfer operator based schemes require high resolution trajectory data, spatio-temporal clustering algorithms have been proven to be very effective for the extraction of coherent sets directly from sparse and possibly incomplete trajectory data. In particular, a discrete representation of the dynamics in terms of a trajectory network forms the basis of a computationally very attractive and flexible framework.

In this contribution, we will review these computational approaches and apply them to a number of example systems, including geophysical flows.

Session CSE VI: 11:00 - 12:30

11:00 - 11:30 Philipp Neumann (HSU)

Molecular-Continuum Flow Simulation with MaMiCo: Where HPC and Data Analytics Meet

Molecular-continuum methods, as referred to in my talk, employ a domain decomposition and compute fluid flow either by means of molecular dynamics (MD) or computational fluid dynamics (CFD) in the subdomains. This enables multiscale investigations of nano- and microflows beyond the limits of validity of classical CFD.

In my talk, I will focus on latest developments in the macro-micro-coupling tool (MaMiCo). MaMiCo enables the coupling of arbitrary CFD and MD solvers, hiding the entire coupling algorithmics from the actual single-scale solvers. After a brief discussion of the limits of the MD method, I will fo- cus on various aspects of the molecular-continuum coupling and its realization in MaMiCo, including parallelization, multi-instance sampling for MD (that is ensemble averaging) and filtering methods that extract smooth responses from the fluctuating MD description to enhance consistency on the side of the contin- uum solver. I will further present preliminary results from a study which aims to generate open boundary force models for MD using machine learning.

11:30 - 12:00 Thomas Slawig (CAU Kiel)

A design pattern approach in PDE-constrained optimization

We extend an existing design pattern approach for dynamical systems to optimal control problems with PDE constraints. Design patterns are abstract concepts that try to formalize problems and solution methods in software design and engineering. They are closely related to the paradigm of object-oriented software development. In the underlying approach by Rouson et al. (ACM Transactions on Math. Software 2010), time-dependent PDEs are considered in a semi-discrete setting as dynamical systems. Then, a unified approach for time integration of dynamical sys-

tems is presented, and implementation details in Fortran and C++ are discussed. The basic design pattern used are an "integrable model" and a "strategy" pattern. In the field of PDE-constrained control, the time integration of the PDE (i.e., state equation) is embedded in an optimization strategy. Usually, the latter involves an adjoint equation and an optimization algorithm. Thus, the whole problem becomes more complicated as the "simple" solution of the underlying PDE itself. We present a design pattern approach for PDE-constrained control problems and discuss the realization in object-oriented software. The idea of our work is on the conceptual level. We are interested in the applicability of object-orientation and design patterns in optimal control; we are not aiming for "the universal PDE control library". Nevertheless, examples in Matlab(R) can and will be given.

12:00 - 12:30 Martin Siebenborn (UHH)

Scalable algorithms for interface identification and shape optimization in function spaces

In many processes described by partial differential equations there is only a small number of materials or parameters to be identified. Typically, the material distribution forms complex contours that can be treated as the variable in a shape optimization approach.

In this talk we consider shape optimization problems as optimization on function spaces via the method of mappings. The focus is on the choice of extension operators, which link a boundary control variable to the set of admissible shape transformations. We investigate conditions on this extension aiming for optimal shapes that preserve the regularity of the reference domain. Towards the definition of a suitable shape space we enrich the optimization problem with a non-linear, semismooth condition, which guarantees local injectivity of transformations. Moreover, it is shown that the coupled system of model and extension equation can naturally be combined with geometric constraints on volume and barycenter of the shape. For the resulting non-linear, coupled optimality system an iterative solution algorithm is proposed which is based on a semismooth Newton method.

The developed methodology is demonstrated in optimal aerodynamical design problems and for the inverse modeling of human skin cells. Here the benefit of the function space perspective of the optimization problem for the mesh quality of discretizations is numerically substantiated.

List of speakers