Doctoral Program
Computational Mathematics
Numerical Analysis and Symbolic Computation

FWF Der Wissenschaftsfonds.

JKU JOHANNES KEPLER UNIVERSITY LINZ

PROGRAM of the DK Computational Mathematics CONCLUDING EVENT, Oct 27-29, 2022, JKU Linz

Thursday, Oct 27

13:30 – 13:35 *Opening*
13:35 – 14:35 Rob Corless *Computational Discovery on Jupyter*
14:35 – 15:05 Koustav Banerjee *Error bounds for the asymptotic expansion of the partition function and its consequences*

COFFEE BREAK

15:30 – 16:30 Anke Wiese *The Exponential Lie Series for Ito Integrals*
16:30 – 17:30 Christoph Hofer *Fast Multipatch Isogeometric Analysis Solvers*

Friday, Oct 28

9:00 – 10:00 Antonella Falini *Matrix Factorization algorithms and Error Functions for the task of Change Detection in HyperSpectral Images*
10:00 – 10:30 Cecilia Schwalsberger *Space-time parallel eddy currents and Kaczmarz methods for adaptive optics*

COFFEE BREAK

11:00 – 12:00 Mohab Safey El Din *Polynomial system solving through Gröbner bases and applications*

LUNCH BREAK

13:30 – 14:30 Nicolas Smoot *Additive Number Theory: An Introduction to Partition Numbers and Their Mysterious Laws*
14:30 – 15:00 Jiayue Qi *Vertex splitting of a loaded tree*

COFFEE BREAK

15:30 – 16:30 Thorsten Hohage *Learned Infinite Elements*
16:30 – 17:00 Amira Meddah *A stochastic hierarchical model for low-grade glioma evolution*

19:00 CONFERENCE DINNER at Promenadenhof, Linz

Saturday, Oct 29

9:00 – 10:00 Lixin Du *Hermite Reduction for D-finite Functions*
10:00 – 10:30 Philipp Nuspl *An extension of C-finite sequences: C^2-finite sequences*

COFFEE BREAK

11:00 – 12:00 Peter Gangl *Space-Time Simulation and Design Optimization of Electric Machines*
Closing

Koustav Banerjee *Error bounds for the asymptotic expansion of the partition function and its consequences*

Study on asymptotics for the partition function began with the work of Hardy and Ramanujan. In this talk, we will see how one can derive the error bounds for the full asymptotic expansion of the partition function starting from Hardy-Ramanujan-Rademacher's formula, which in turn, finally gives an infinite family of inequalities. Among its many other application, we shall focus on log-concavity, higher order Turan inequalities, higher order Laguerre inequalities for the partition function.

Rob Corless *Computational Discovery on Jupyter*

Recently, with Neil Calkin and Eunice Chan, I have published an Online Educational Resource (OER) entitled "Computational Discovery on Jupyter." This is freely available online now at the link below, and I will give the talk directly from the online version. It is now also in the process of being turned into a book to be published by SIAM. The material is aimed at graduating high-school students and entering University students in North America, but tries hard not to include anything from the usual curriculum. Instead, it tries to get the student/participant to be able to appreciate (and perhaps contribute to the solution of) open problems as soon as possible.

The table of contents is as follows: Fibonacci Numbers, Continued Fractions, Rootfinding, Fractals & Julia sets, Bohemian matrices, Mandelbrot polynomials and matrices, and the Chaos game representation. We have several appendices, and solutions to almost all the exercises (which are called Activities).

The main interest for this audience might be the technology we used (Jupyter Book, built on top of Jupyter Notebooks using Python) but there are several open problems we might profitably discuss.

I even claim to be able to show you new things about Fibonacci numbers. Now, while I can prove that these things are true, it is a different matter indeed to prove that they are actually new! But I am sure that if *anyone* knows these facts already, they will be in the audience; so I look forward to finding out for sure.

Lixin Du *Hermite Reduction for D-finite Functions*

Ostrogradsky-Hermite reduction is a symbolic integration technique that reduces rational functions to integrands with only simple poles. Hermite reduction was extended by Trager from the field of rational functions to the field of algebraic functions via integral bases. Trager's Hermite reduction solved the integration problem for algebraic functions. This work was extended to Fuchsian D-finite functions. We remove the Fuchsian restriction and present Hermite reduction for general D-finite functions via integral bases. It reduces the pole orders of integrands at finite places, but may not reduce to simple poles as in the algebraic and Fuchsian D-finite cases. Instead of using the polynomial reduction, we develop Hermite reduction at infinity to reduce the pole order of D-finite functions at infinity via local integral bases at infinity. Combining Hermite reduction at finite places and at infinity, we obtain a reduction-based telescoping algorithm for D-finite functions in two variables.

Antonella Falini *Matrix Factorization algorithms and Error Functions for the task of Change Detection in HyperSpectral Images*

When hyperspectral images are analyzed, a big amount of data, representing the reflectance at hundreds of wavelengths, needs to be processed and therefore, specific matrix factorization algorithms are used to express the original problem in suitable subspaces. In the present talk, we show some recent results derived also by using spatial and spectral functions to compute a lower rank approximation of the original matrix and to measure the reconstruction error between the input image and the approximate one, with applications to the task of change-detection.

Peter Gangl *Space-Time Simulation and Design Optimization of Electric Machines*

Electric machines can often be modeled by the magneto-quasi-static approximation of Maxwell's equations in two space dimensions. We consider the simulation of a rotating electric machine by means of a space-time finite element method where the rotation is captured by the tetrahedral space-time mesh. We derive the shape derivative as well as the topological derivative for a given cost function with respect to a perturbation of the (spatial) geometry and present corresponding design optimization algorithms for moving domains in space-time. Here, it is important to note that the optimized geometry is moving, but must not change its shape over time. Finally, we present numerical results for the optimization of a synchronous reluctance machine and give an outlook towards the use of higher order topological derivatives to accelerate optimization algorithms.This work is based on joint work with Alessio Cesarano and Nepomuk Krenn (RICAM), Olaf Steinbach and Mario Gobrial (TU Graz) and Charles Dapogny (Univ. Grenoble).

Christoph Hofer *Fast Multipatch Isogeometric Analysis Solvers*

In the first part of the talk, we investigate fast solvers for large-scale linear systems of algebraic equations arising from Isogeometric Analysis (IgA) of diffusion problems with heterogeneous diffusion coefficients on multipatch domains. We investigate the adaption of the Dual-Primal Finite Element Tearing and Interconnecting (FETI-DP) method to IgA, called Dual-Primal IsogEometric Tearing and Interconnecting (IETI-DP) method. We consider the cases where we have matching, and non-matching meshes on the interfaces. We use ideas from the finite element case to formulate the corresponding IETI-DP method, called dG-IETI-DP. Numerical results for two- and three-dimensional domains are presented.

In the second part of the talk, we construct and investigate fast solvers for large-scale linear systems arising from the application of IgA to parabolic diffusion problems. We consider decompositions of the space-time cylinder into time slabs, where each slab is again decomposed into several space-time patches. The aim is to investigate fast solvers, which are based on a time parallel multigrid method. We present two strategies for an efficient implementation of the smoother. The main idea is a decomposition of the space-time problem into a series of spatial problems via an eigen-decomposition. The proposed algorithms are well suited for parallelization.

In the third and last part of the talk, I give an overview of my current work at RISC-Software GmbH and the some of the projects I am involved.

Thorsten Hohage *Learned Infinite Elements*

We discuss the numerical solution of scalar time-harmonic wave equations on unbounded domains which can be split into a bounded interior domain of primary interest and an exterior domain with separable geometry. To compute the solution in the interior domain, approximations to the Dirichlet-to-Neumann (DtN) map of the exterior domain have to be imposed as transparent boundary conditions on the artificial coupling boundary. Although the DtN map can be computed by separation of variables, it is a nonlocal operator with dense matrix representations, and hence computationally inefficient. Therefore, approximations of DtN maps by sparse matrices, usually involving additional degrees of freedom, have been studied intensively in the literature using a variety of approaches including different types of infinite elements, local nonreflecting boundary conditions, and perfectly matched layers. The entries of these sparse matrices are derived analytically, e.g., from transformations or asymptotic expansions of solutions to the differential equation in the exterior domain. In contrast, we propose to “learn” the matrix entries from the DtN map in its separated form by solving an optimization problem as a preprocessing step.

We show that the approximation quality of learned infinite elements improves exponentially with increasing number of infinite element degrees of freedom, which is confirmed in numerical experiments. These numerical studies also show that learned infinite elements outperform state-of-the-art methods for the Helmholtz equation. At the same time, learned infinite elements are much more flexible than traditional methods as they, e.g., work similarly well for exterior domains involving strong reflections. As the main motivating example we study the atmosphere of the Sun, which is strongly inhomogeneous and exhibits reflections at the corona.

Amira Meddah *A stochastic hierarchical model for low-grade glioma evolution*

A stochastic hierarchical model of the evolution of low-grade gliomas is proposed. Starting with the description of cell motion using piecewise diffusion Markov processes (PDifMPs) at the cellular level, we derive an equation for the transition probability density of this Markov process using the generalized Fokker-Planck equation. Then, a macroscopic model is derived via the parabolic limit and the Hilbert expansions in the equations of moments. After setting up the model, we perform several numerical tests to study the role of local characteristics and the extended generator of the PDifMP in the process of cell movement and tumor progression.

Philipp Nuspl *An extension of C-finite sequences: C^2-finite sequences*

We define a class of sequences which satisfy a linear recurrence with coefficients that, in turn, satisfy a linear recurrence with constant coefficients themselves, i.e., are C-finite. These C^2-finite sequences form a ring and satisfy additional computational properties. It turns out that the algorithmic aspects are much more involved and are related to difficult problems in number theory. Restricting the leading coefficient of the recurrences we can avoid some of these problems and we obtain the computable ring of simple C^2-finite sequences. Additionally, we present an implementation of C^2-finite sequences in the computer algebra system SageMath.

Jiayue Qi *Vertex splitting of a loaded tree*

We introduce an operation on a type of tree which is defined to be the loaded trees in the talk. Also, we claim that it is the graphical characterization of the linear reduction on monomials in the Chow ring of the moduli space of stable marked curves of genus zero.

Mohab Safey El Din *Polynomial system solving through Gröbner bases and applications*

Gröbner bases algorithms and computations are versatile tools for solving exactly non-linear algebraic equations. They can be used in a wide range of important and challenging applications ranging from e.g. information theory and security (coding theory, cryptology) - where base fields are finite fields - to applications in engineering sciences (biology, chemistry, robotics).

In this talk, we will recall basic definitions and properties of Gröbner bases, and explain how these properties can be used to solve polynomial systems (in a broad sense). Next, a few glimpse on algorithmic aspects, computational issues and implementation bottlenecks will be given. Topical applications in cryptography will be reviewed. Challenging applications in robotics, on which numerical methods tend to fail, will illustrate the potential of Gröbner bases for engineering sciences. Practical experiments and reports will use the C library msolve and its companion AlgebraicSolving.jl Julia package, authored by Berthomieu, Eder and Safey El Din.

Cecilia Schwalsberger *Space-time parallel eddy currents and Kaczmarz methods for adaptive optics*

In this overview talk, I will give a comprehensive summary of the topics we have worked on during my PhD. The first project concerned solving the eddy current equation parallel in time; results for an induction furnace model are included. The second part is about using Kaczmarz methods for solving the mirror fitting problem in adaptive optics for telescopes. For this application the Kaczmarz approach is coupled with a quasi-Monte-Carlo discretication in a unique way.

Nicolas Smoot *Additive Number Theory: An Introduction to Partition Numbers and Their Mysterious Laws*

Additive number theory is concerned with the study of how a given whole number n may be expressed a sum of other whole numbers. Such an expression is called a partition of n if the ordering of the summands is considered irrelevant. For example, the number 4 has 5 different partitions: 4, 3+1, 2+2, 2+1+1, 1+1+1+1. The partition number of 4, denoted p(4), is then 5. In 1918 Ramanujan discovered that p(n) exhibits an extraordinary arithmetic structure. In the century since then, an enormous amount of research has been devoted to p(n) and more restrictive partition functions. Much of this research has come from work at JKU. We will briefly review p(n), its arithmetic properties, analogous properties of closely related functions, work done at JKU and even within the DK program, and standing problems. This talk will be accessible to a broad audience.

Anke Wiese *The Exponential Lie Series for Ito Integrals*

We consider stochastic differential systems driven by a multi-dimensional Wiener process (more generally by continuous semimartingales) and governed by non-commuting vector fields. The flow map describes the transport of the initial condition to the solution of the differential equation at a future time. We prove that the logarithm of the flow map is a Lie series. This is an important property for the development of strong Lie group integration schemes that ensure approximate solutions themselves lie in any homogeneous manifold on which the solution evolves.