2nd SFB International Workshop

"Taming Complexity in Partial Differential Systems"

April 19th – April 21st, 2023

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organized by

Jens Markus Melenk (TU Wien), **Ilaria Perugia** (University of Vienna),
Dirk Praetorius (TU Wien), and **Joachim Schöberl** (TU Wien)

Schedule

All the talks and the registration will take place in the Sky Lounge on the 12th floor of the Faculty of Mathematics of the University of Vienna (Oskar-Morgenstern-Platz 1, 1090 Vienna).

Wednesday, April 19th 2023

9:30 - 10:15 Registration

10:15 - 10:30 Opening remarks

10:30 - 11:15 **Angela Kunoth** (Universität zu Köln, Germany)
Adaptive Approximations for PDE-Constrained Parabolic Control Problems

11:15 - 11:45 Coffee break

11:45 - 12:30 **Paul Houston** (University of Nottingham, UK)
hp-Version Polytopic Discontinuous Galerkin Methods for Radiation Transport Problems

12:30 - 14:30 Lunch break (see some suggestions about food shops and restaurants at the end of this handout)

14:30 - 15:15 **Valeria Simoncini** (University of Bologna, Italy)
Sketching meets Krylov in space-time

15:15 - 16:00 **Théophile Chaumont-Frelet** (Inria, Université Côte d'Azur, France)
Efficient discretization of high-frequency Helmholtz problems with semi-classical Gabor wavelets

16:00 - 16:45 Coffee break

16:45 - 19:00 Poster session with reception (details at the end of this handout)

Thursday, April 20th 2023

9:00 - 9:45 **Paola Antonietti** (Politecnico di Milano, Italy)
Discontinuous Galerkin methods on polyhedral grids for the numerical modeling of neurodegenerative diseases

9:45 - 10:30 **Emmanuil Georgoulis** (Heriot-Watt University, UK; National Technical University of Athens, Greece)
Hypococercivity-preserving Galerkin discretisation for kinetic equations

10:30 - 11:00 Coffee break

11:00 - 11:45 **Luca Gerardo Giorda** (Johannes Kepler Universität Linz, Austria)
TBA

11:45 - 12:30 **Andrea Bonito** (Texas A&M University, USA)
Approximating partial differential equations with incomplete information

12:30 - 14:30 Lunch break (see some suggestions about food shops and restaurants at the end of this handout)

14:30 - 15:15 **Lorenzo Pareschi** (Università di Ferrara, Italy)
Breaking complexity in high-dimensional kinetic and mean-field equations

15:15 - 16:00 **Herbert Egger** (Johannes Kepler Universität Linz, Austria)
Asymptotic analysis for instationary gas transport in pipe networks

16:00 - 16:30 Coffee break

16:30 - 17:15 **David Silvester** (University of Manchester, UK)
Error estimation and adaptivity for stochastic collocation finite elements

From 19:00 Social dinner (details at the end of this handout)

Friday, April 21st 2023

9:00 - 9:45 **Claudio Canuto** (Politecnico di Torino, Italy)
Convergence and Optimality for a class of Adaptive Virtual Element Methods

9:45 - 10:30 **Gianluigi Rozza** (SISSA, Italy)
Reduced Order Modelling in Computational Fluid Mechanics: state of the art, challenges and applications

10:30 - 11:00 Coffee break

11:00 - 11:45 **Robert Scheichl** (Universität Heidelberg, Germany)
Multiscale Spectral Generalised Finite Element Methods

11:45 - 12:30 **Barbara Wohlmuth** (Technische Universität München, German)
Polynomial-type surrogates for algorithmic efficiency

12:30 - Closing remarks and lunch (see some suggestions about food shops and restaurants at the end of this handout)

List of abstracts

Paola Antonietti (Politecnico di Milano, Italy)

Discontinuous Galerkin methods on polyhedral grids for the numerical modeling of neurodegenerative diseases

Abstract: Neurodegenerative diseases (NDs) are complex disorders that primarily affect the neurons in the brain and nervous system, leading to progressive deterioration and loss of function over time. A common pathological hallmark among different NDs is the accumulation of disease–specific misfolded aggregated prionic proteins in different areas of the brain (Aβ and tau in Alzheimer's disease, α–synuclein in Parkinson's disease). In this talk, we discuss the numerical modeling of the misfolding process of α–synuclein in Parkinson's disease. To characterize the progression of misfolded proteins across the brain we consider a suitable mathematical model (based on Fisher– Kolmogorov equations). For its numerical discretization, we propose and analyze a high-order discontinuous Galerkin method on polyhedral grids (PolyDG) for space discretization coupled with a Crank-Nicolson scheme to advance in time. Numerical simulations in patient-specific brain geometries reconstructed from magnetic resonance images are presented. In the second part of the talk, we introduce and analyze a PolyDG method for the semidiscrete numerical approximation of the equations of Multiple-Network Poroelastic Theory (MPET) in the dynamic formulation. The MPET model can comprehensively describe functional changes in the brain considering multiple scales of fluids and can be regarded as a preliminary attempt to model the perfusion in the brain. In this context, the cerebrospinal fluid transport plays an important role as a mechanism for waste removal (clearance) from the central nervous system, particularly important in Alzheimer's disease. We present and analyze the numerical approach and we present simulations in three dimensional patient-specific geometries.

Andrea Bonito (Texas A&M University, USA)

Approximating partial differential equations with incomplete information

Abstract: The problem of learning an unknown function from given data, i.e., construct an approximation to the function that predicts its values away from the data is ubiquitous in modern science. There are numerous settings for this learning problem depending on what additional information is provided about the unknown function, how the accuracy is measured, what is known about the data and data sites, and whether the data observations are polluted by noise.

In the first part of the talk, we provide a mathematical description of optimal performances in the presence of a model class assumption. Under standard model class assumptions, we show that a near optimal recovery can be found by solving a certain discrete over-parameterized optimization problem with a penalty term. This indicates the advantage of over-parameterization which is commonly advocated in modern machine learning.

In the second part of the talk, we consider the specific case where the learning problem consists of determining the solutions to a partial differential equation when there is insufficient information to determine a unique solution. This lack of infor-

mation is alleviated by finitely many linear measurements of the solution. Our main example is the Poisson boundary value problem without boundary data. We present and discuss the near optimal property of a recovery algorithm in this context.

Claudio Canuto (Politecnico di Torino, Italy)

Convergence and Optimality for a class of Adaptive Virtual Element Methods

Abstract: We consider discretizations of elliptic boundary-value problems, based on nonconforming triangular or quadrilateral meshes generated by successive bisections without completion. The key notion of global index of a hanging node establishes a hierarchical organization of the nonconformity in the mesh. Any element carrying hanging nodes on its boundary is equipped with a structure of Virtual Element of fixed degree.

We design a two-stage adaptive virtual element algorithm, based on a stabilization-free a posteriori error estimator, which alternates data approximation and solution approximation with increasing accuracy. We prove the convergence of the inner and outer loops, establish the optimality of the adaptive procedure in suitable approximation classes, and illustrate some representative numerical experiments.

These results have been obtained through collaborations with L. Beirão da Veiga, R.H. Nochetto, G. Vacca, M. Verani, and with D. Fassino.

Théophile Chaumont-Frelet (Inria, Université Côte d'Azur, France)

Efficient discretization of high-frequency Helmholtz problems with semi-classical Gabor wavelets

Abstract: The accurate simulation of high-frequency wave propagation problems in heterogeneous media is crucial for many scientific applications central to our society. To maintain a constant accuracy as the frequency increases, finite element methods require (at least) a constant number of degrees of freedom per wavelength, leading to a total number of degrees of freedom scaling as k^d, d being the spatial dimension. In this talk, I will propose to replace polynomial shape functions by semi-classical Gabor wavelets. Specifically, I will show that these new shape functions (i) provide a constant accuracy in the high-frequency regime with only $k^{d-1/2}$ degrees of freedom, (ii) can operate in general heterogeneous media, and (iii) lead to a sparse linear system. I will also present preliminary numerical examples in one-dimensional benchmarks that illustrate the theoretical estimates and suggest that Gabor wavelets can lead to efficient discretization methods for two- and three-dimensional problems.

This is a joint work with V. Dolean and M. Ingremeau.

Herbert Egger (Johannes Kepler Universität Linz, Austria)

Asymptotic analysis for instationary gas transport in pipe networks

Abstract: We consider the transport of gas in long pipes and pipeline networks for which the dynamics are dominated by friction at the pipe walls. The governing equations can be formulated as an abstract dissipative Hamiltonian system which allows us to derive perturbation bounds by means of relative energy estimates. As particular consequences, we obtain stability with respect to initial conditions and model parameters and quantitative asymptotic estimates in the high friction

limit. Our results cover the flow in a single pipe but also generalize to pipe networks. Moreover, they allow to formulate an asymptotic preserving numerical scheme.
Joint work with Jan Giesselmann, Teresa Kunkel, and Nora Philippi.

Emmanuil Georgoulis (Heriot-Watt University, UK; National Technical University of Athens, Greece)

Hypococercivity-preserving Galerkin discretisation for kinetic equations

Abstract: Degenerate differential evolution PDE problems are often characterised by the explicit presence of diffusion/dissipation in some of the spatial directions only, yet may still admit decay properties to some long time equilibrium. Classical examples include the inhomogeneous Fokker-Planck equation, Boltzmann equation with various collision kernels, systems of equation arising in micromagnetism or flow vorticity modelling, etc. In the celebrated AMS memoir "Hypocoercivity", Villani introduced the concept of hypocoercivity to describe a framework able to explain decay to equilibrium in the presence of dissipation in some directions only. The key technical idea involved is to exploit certain commutators to overcome the degeneracy of dissipation. I will present some results and ideas on the development of numerical methods which preserve the hypocoercivity property upon discretisation. Therefore, such numerical methods will be suitable for arbitrarily long-time simulations. The methods are constructed by addressing the key challenge of lack of commutativity between differentiation and discretisation in the context of mesh-based Galerkin-type numerical methods via the use of carefully constructed non-conforming weak formulations of the underlying evolution problems.

Paul Houston (University of Nottingham, UK)

hp-Version Polytopic Discontinuous Galerkin Methods for Radiation Transport Problems

Abstract: In this talk we develop hp–version discontinuous Galerkin finite element methods (DGFEMs) for the discretization of the radiation transport problem on general (spatial) computational meshes consisting of polygonal/polyhedral (polytopic) elements. Our particular interest is the application to medical treatment planning in clinical radiotherapy. Here we study both the stability and a priori error analysis of the proposed scheme. The implementation is based on exploiting a nodal approximation in energy and angle, together with fast numerical integration techniques on the spatial polytopic mesh; this approach leads to a highly parallelisable algorithm whereby a large number of linear transport solves must be computed. Numerical experiments are presented to highlight the accuracy of the proposed method, as well as to benchmark with more standard kinetic Monte Carlo simulations.

Angela Kunoth (Universität zu Köln, Germany)

Adaptive Approximations for PDE-Constrained Parabolic Control Problems

Abstract: Numerical solvers for PDEs have matured over the past decades in efficiency, largely due to the development of sophisticated algorithms based on closely intertwining theory with numerical analysis. Consequently, systems of PDEs as they arise from optimization problems with PDE constraints also have become more and more tractable.
Optimization problems constrained by a parabolic evolution PDE are challenging from a computational point of view: They

require to solve a system of PDEs coupled globally in time and space. For their solution, time-stepping methods quickly reach their limitations due to the enormous demand for storage. An alternative approach is a full space-time weak formulation of the parabolic PDE which allows one to treat the constraining PDE as an operator equation without distinction of the time and space variables. An optimization problem constrained by a parabolic PDE in full space-time weak form leads to a coupled system of corresponding operator equations which is, of course, still coupled globally in space and time.
For the numerical solution of such coupled PDE systems, adaptive methods appear to be most promising, as they aim at distributing the available degrees of freedom in an a-posteriori-fashion to capture singularities in the data or domain. Employing wavelet schemes, we can prove convergence and optimal complexity. The theoretical basis for proving convergence and optimality of wavelet-based algorithms for such type of coupled PDEs is nonlinear approximation theory and the characterization of solutions of PDEs in Besov spaces.
Wavelet schemes are, however, more involved when it comes to implementations compared to finite element approximations. I will finally address corresponding ideas and results.

Lorenzo Pareschi (Università di Ferrara, Italy)

Breaking complexity in high-dimensional kinetic and mean-field equations

Abstract: In many fields, from classical physics and engineering to social sciences and artificial intelligence, solving high-dimensional problems in the form of kinetic and/or mean-field PDEs is crucial. In this talk, we will review recent advancements in the numerical solution of such problems, using both deterministic and stochastic techniques. Our focus will be on key aspects such as computational complexity, conservation properties, and uncertainty quantification.

Gianluigi Rozza (SISSA, Italy)

Reduced Order Modelling in Computational Fluid Mechanics: state of the art, challenges and applications

Abstract: We provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD). Efficient parametrisations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments in CFD include: (i) a better use of stable high fidelity methods, to enhance the quality of the reduced model too, and allowing to incorporate turbulence models and increasing the Reynolds number; (ii) more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; (iii) the improvements of the certification of accuracy based on residual based error bounds and of the stability factors, as well as the guarantee of the stability of the approximation with proper space enrichments. All the previous aspects are quite relevant in CFD problems to focus on real time simulations for complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation and uncertainty quantification. Model flow problems will focus on few benchmarks, as well as on simple fluid-structure interaction problems and shape optimisation, applied to some industrial and environmental problems of interest.

Robert Scheichl (Universität Heidelberg, Germany)

Multiscale Spectral Generalised Finite Element Methods

Abstract: In this talk, I will present an efficient generalized finite element method with optimal (multiscale spectral) local approximation spaces (MS-GFEM) for PDEs with heterogeneous coefficients, providing rigorous error estimates for the fully discrete method. The local approximation spaces are constructed from local eigenvalue problems solved on some sufficiently fine finite element mesh with mesh size h. The error bound of the discrete MS-GFEM approximation is proved to converge as h tends to 0 towards that of the continuous MS-GFEM approximation, which was shown to decay nearly exponentially in previous works. Moreover, even for fixed mesh size h, a nearly exponential rate of convergence of the local approximation errors with respect to the dimension of the local spaces is established. The method can also be used as an effective preconditioner in an iterative solver with a 'tuneable' convergence rate. On the practical side, an efficient and accurate method for solving the discrete eigenvalue problems is proposed by incorporating the discrete-harmonic constraint directly into the eigenproblem via a Lagrange multiplier approach. Numerical experiments that confirm the theoretical results and demonstrate the effectiveness of the method are presented for a second-order elliptic problem, for a large-scale problem of linear elasticity in composite aerospace applications and for a high-frequency heterogeneous Helmholtz problem. Even in this last example, a quasi-optimal and nearly exponential (wavenumber-explicit) global convergence of the method can be theoretically proved, provided the size of the subdomains is $O(1/k)$ (where k is the wavenumber).

David Silvester (University of Manchester, UK)

Error estimation and adaptivity for stochastic collocation finite elements

Abstract: A multilevel adaptive refinement strategy for solving linear elliptic partial differential equations with random data is discussed herein. The strategy extends the a posteriori error estimation framework introduced by Guignard & Nobile in 2018 to cover problems with a *nonaffine* parametric coefficient dependence. A suboptimal, but nonetheless reliable and convenient implementation of the strategy involves approximation of the decoupled PDE problems with a common finite element approximation space. Computational results obtained using such a *single-level* strategy are presented in the first half of the talk. Results obtained using a potentially more efficient *multilevel* approximation strategy, where meshes are individually tailored, are discussed in the second half. Our results demonstrate that the optimal convergence rates can be achieved, but only when solving specific types of problems. The codes used to generate the numerical results are available on GitHub. This is joint work with Alex Bespalov and Feng Xu.

Valeria Simoncini (University of Bologna, Italy)

Sketching meets Krylov in space-time

Abstract: Linear algebraic problems such as Sylvester matrix equations and their generalizations have classically played an important role in the analysis of dynamical systems. More recently, matrix equations have emerged as a natural linear algebra framework for the discretized version of (systems of) deterministic and stochastic partial differential equations

(PDEs), and new challenges have arisen. The use of matrix-oriented Krylov methods is crucial for the solution of these equations when dealing with large matrices generated by fine discretizations and tensor bases. In spite of their advantages over standard vector-oriented iterative solvers, computational costs and/or memory requirements can still hinder the full potential of matrix-oriented solvers. In this talk we show that very recently developed sketching strategies can be adapted to Krylov spaces for these problems, so as to dramatically lower memory and computational requirements compared with advanced well established second generation Krylov schemes. We will illustrate these properties by means of computational experiments with data stemming from space-time discretizations of time dependent PDEs.
This talk is based on joint works with Julian Henning, Davide Palitta, Marcel Schweitzer, Karsten Urban.

Barbara Wohlmuth (Technische Universität München, Germany)

Polynomial-type surrogates for algorithmic efficiency

Abstract: In this talk, we discuss several aspects of surrogate approximation techniques to reduce memory in case of history dependent PDE solutions, to facilitate the re-assembling in matrix-free large scale applications or to speed up the classical element-wise assembling procedure for IGA. Theoretical and performance aspects are discussed. A matrix-free block ILU(0) smoother, the assembling of IGA and low order large scale matrix-free FEs are used to demonstrate the flexibility of surrogate polynomial approximations. Rational approximations allow to reformulate fractional order PDEs in time or space as integer order systems of moderate size. Numerical examples illustrate the performance with respect to accuracy, scaling and run-time.

Poster session

A poster session with a reception will take place **from 16:45 to 19:00 on Wednesday, April 19th**. During the poster session, results and work in progress from the Viennese community will be presented. Each of these results involves one or several members of the SFB 65 Project **Taming Complexity in Partial Differential Systems**.

Project Part 0 (Coordination Part of the SFB)
Poster on *Low-rank tensor approximation from incomplete data and under constraints*
presented by **Stanislav Budzinskiy** (University of Vienna)

Project Part 1 (Large-time behavior of continuous dissipative systems - Anton Arnold)
Poster on *WKB-based methods for the 1D stationary highly oscillatory Schrödinger equation*
presented by **Jannis Körner** (TU Wien)

Project Part 2 (Large-time behavior of discrete dissipative systems - Ansgar Jüngel)
Poster on *Long-time behaviour for finite volume schemes for Fokker-Planck equations*
presented by **Katharina Schuh** (TU Wien)

Project Part 3 (Structure preserving variational discretisation via optimal transport - Jan Maas & Julian Fischer)

Poster on *Interacting particle dynamics: an approach via optimal transport*

presented by **Lorenzo Dello Schiavo** (IST Austria)

Poster on *Density fluctuations of interacting particle systems via SPDEs*

presented by **Jonas Ingmanns** (IST Austria)

Project Part 5 (Time dependent (magnetic) Schrödinger equations - Norbert J. Mauser)

Poster on *GHD: Generalized HydroDynamics, a model for quasi-1D quantum systems*

presented by **Igor Mazets** (University of Vienna and TU Wien) and **Hans Peter Stimming** (University of Vienna)

Poster on *Efficient numerics for dynamic Bose Einstein Condensates*

presented by **Jan-Frederik Mennemann** (University of Vienna)

Project Part 6 (High order numerical methods for nonlocal operators - Jens Markus Melenk)

Poster on *Numerical methods for non-local operators*

presented by **Björn Bahr** (TU Wien), **Markus Faustmann** (TU Wien), **Jens Markus Melenk** (TU Wien), and **Alexander Rieder** (TU Wien)

Project Part 7 (Problem-adapted discretisations of wave equations - Ilaria Perugia)

Poster on *Geometry-based approximation of waves in complex domains*

presented by **Monica Nonino** (University of Vienna)

Project Part 8 (Coupling in computational micromagnetics - Dirk Praetorius & Michael Feischl)

Poster on *Optimal cost of AFEM for linear elliptic PDEs*

presented by **Ani Miraçi** (TU Wien) and **Julian Streitberger** (TU Wien)

Poster on *High-Dimensional and Adaptive Approximation in Computational Micromagnetics*

presented by **Hubert Hackl** (TU Wien) and **Andrea Scaglioni** (TU Wien)

Project Part 10 (Automated discretization in multiphysics - Joachim Schöberl)

Poster on *NGsolve*

presented by **Joachim Schöberl** (TU Wien)

Poster on *Distributional curvatures of Regge metrics*

presented by **Michael Neunteufel** (TU Wien)

Project Part 11 (Multiphysics effects in solids - Ulisse Stefanelli)

Poster on *A global variational approach to elastodynamics*

presented by **Riccardo Voso** (University of Vienna)

Project Part 12 (Nonlocal challenges in continuum mechanics - Elisa Davoli)

Poster on *Stochastic homogenization in micromagnetics*

presented by **Lorenza D'Elia** (TU Wien)

Project Part 13 (Atmospheric Flow Models for Cloudy Air - Sabine Hittmeir & Christian Schmeiser)

Poster on *Discontinuous Galerkin for Moist Air*

presented by **Henry von Wahl** (University of Vienna)

Project Part 14 (Emergent properties in models for collective dynamics - Sara Merino Aceituno & Christian Schmeiser)

Poster on *Emergent properties in models for collective dynamics*

presented by **Raphael Winter** (University of Vienna)

Food shops and restaurants nearby

In the building hosting the Faculty of Mathematics of the University of Vienna there is a **mensa** (closing at 13:30) having also a **small bar** (closing at 14:00). You can find them both on the first floor of the Faculty of Mathematics: from the Sky Lounge, take any of the elevators to the first floor, then take the corridor in front of you and walk until the end of it.

In order to see the menu of the day, you can use the website www.mensen.at and select in the dropdown menu (*Standort auswählen*) the option *Uni Wien Mensa OMP*.

There are two **supermarkets** near the Faculty of Mathematics:

- BILLA, located in Schlickgasse 6;
- SPAR Gourmet, located in Servitengasse 1.

There are lots of **small take-away shops** in the area (with a small number of seating places). Among others:

- a Turkish place (Sentepe, in Bergasse 29);
- a place selling bowls and vegetarian hamburgers (Plain Kitchen Vienna, in Bergasse 25);
- a place selling soups and curry dishes (Suppenwirtschaft, in Servitengasse 6).

If you prefer **restaurants**, we would suggest to call and book in advance. Among others, we would recommend:

- an Italian pizzeria (Riva Türkenstraße), at the corner between Schlickgasse and Türkenstraße (tel: +43 1 310 2088);
- the restaurant Porzellan Lounge in Servitengasse 2 (tel: +43 1 315 6363);
- an Austrian restaurant (Gasthaus Rebhuhn), located in Berggasse 24 (tel: +43 1 319 5058);

- a restaurant selling Asian specialties (SteirAsia), in Servitengasse 3 (tel: +43 1 346 3875).

Also at walking distance you can find *La Mercerie*, a French café, located in Berggasse 25.

On the website of the Workshop (**bit.ly/sfb-lunch**) you can find links to the websites of all the commercial activities mentioned above.

Social dinner

The social dinner will take place starting from **19:00 on Thursday, April 20th** at the restaurant **Zwölf Apostelkeller**, located in **Sonnenfelsgasse 3, 1010 Vienna**.

The dinner will be a buffet, with specialties from Viennese cuisine (also with some vegetarian dishes). The dinner is offered by the workshop; you will only have to pay for alcoholic beverage by yourself (if you want any) since we cannot cover this with money from grants of the Austrian Science Fund (FWF).

You can use the link **bit.ly/sfb-social-dinner** for some pictures of the restaurant and for directions from the workshop venue and from the hotels of the workshop.

This workshop is funded by the SFB 65 Project **Taming Complexity in Partial Differential Systems**. This is a consortile venture, currently joining 17 applied-PDEs groups at the **University of Vienna**, **TU Wien**, and the **Institute of Science and Technology (IST) Austria**. The project is funded by the **Austrian Science Fund (FWF)** with additional financial contributions from the 3 involved research institutions.

You can find further details about our activities at the website sfb65.univie.ac.at