Swiss Numerics Day 2023

June 7, 2023

UNIVERSITÄT BERN

Time	Program		
9.30	Registration in front of Lecture Hall A6		
10.00	Welcome		*Lecture Hall A6*
10.05	**Plenary talk** – Prof. Andreas Veeser *Rate-optimal adaptive finite element methods with error-dominated oscillation*		*Lecture Hall A6*
11.00	Coffee break		
	Contributed session 1		
	Lecture Hall B5 Chair: Daniel Kressner	*Lecture Hall B6* Chair: Christoph Schwab	*Lecture Hall B7* Chair: Michael Multerer
11.30	Foivos Alimisis – *New geometric approaches in solving eigenvalue problems*	Nis-Erik Bohne – *The pressure-wired Stokes element: An inf-sup stable generalization of the Scott-Vogelius element*	Ricardo Reyes – *Reduced order models for time-dependent problems using the Laplace transform*
12.00	Dimosthenis Pasadakis – *Learning graph Laplacian matrices via maximum likelihood*	Wouter Tonnon – *Semi-Lagrangian Finite Element Exterior Calculus for Incompressible flows*	Ramona Häberli – *Overcoming the order barrier two in splitting methods when applied to semi-linear parabolic problems with nonperiodic boundary conditions*
12.30	Silvio Barandun – *Edge modes in subwavelength resonators in one dimension*	Martin Licht – *Towards finite element exterior calculus on manifolds*	
13.00	**Poster session** and lunch break		
	Contributed session 2		
	Lecture Hall B5 Chair: Fabio Nobile	*Lecture Hall B6* Chair: Marcus Grote	*Lecture Hall B7* Chair: Helmut Harbrecht
14.00	Junming Duan – *Machine learning enhanced real-time aerodynamic forces prediction based on sparse pressure sensor inputs*	Eugen Bronasco – *Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling*	Joost Opschoor – *Constructive deep neural network approximations of weighted analytic solutions to partial differential equations in polygons*
14.30	Tim De Ryck – *Weak physics-informed neural networks for approximating entropy solutions of hyperbolic conservation laws*	Lisa Gaedke-Merzhäuser – *Spatio-Temporal Bayesian Modeling at Scale*	Remo von Rickenbach – *Compression of Boundary Integral Operators Discretised by Anisotropic Wavelet Bases*
15.00	Coffee break		
15.30	**Plenary talk** — Prof. Thomas Richter *Modeling and Simulation of Temporal Multiscale Problems*		*Lecture Hall A6*
16.30	Closing		

Venue

SND 2023 is an on-site event at the University of Bern. The conference will be held at the Exact Sciences building, Lecture Hall A6, which is within 5 minutes walking distance from the main train station.

Abstracts of plenary talks

Rate-optimal adaptive finite element methods with error-dominated oscillation

Prof. Andreas Veeser, Università degli studi di Milano, Italy

Kreuzer/Veeser '21 propose an approach to a posteriori error analysis, where the data oscillation is bounded in terms of the error. Consequently, the resulting estimator is fully equivalent to the error, not only up to some oscillation terms.

In this talk we will review this approach, discuss its use in adaptive algorithms proving convergence and rate optimality of the latter. Doing so, we shall highlight the differences to previous approaches.

This a joint work with Christian Kreuzer (TU Dortmund).

Modeling and Simulation of Temporal Multiscale Problems

Prof. Thomas Richter, University of Magdeburg, Germany

The coupling of different temporal scales is common in many application problems. One classic example is the weathering of mechanical structures like bridges, a process that takes decades that it is, however, affected by short term influences such as traffic, wind or stretching by daily and yearly temperature alteration. The problem is two-way coupled as material change could cause a shift of resonance regimes with a drastic influence on the fast scale. Another example is the growth of atherosclerotic plaques in blood vessels, a bio/chemical mechanism that causes material transformation and growth within the vessel wall in a time-span of months, but that is strongly affected by the mechanical forces arising from the pulsating blood flow in a fluid-solid interaction system. Narrowing of the blood vessel by growth will in term also affect the fast scale by changing the overall flow pattern.

These slow-scale / fast-scale problems have in common that they are two-way coupled processes and that we are usually interested in the slowly evolving scale only. A resolved simulation of all scales is not feasible. A year comprises 30 million heart cycles, a corresponding resolved fluid-solid simulation is out of bounds.

Based a replacement of the fast-scale by isolated local problems which are periodic in time, we describe and analyse temporal multiscale schemes for the efficient simulation of the slow-scale variable. For simplified classes of equations, we will show convergence of the resulting multiscale method with regard to all discretization and modelling parameters. The main issues of a practical implementation are on the one hand the efficient choice of all parameters, e.g. based on a posteriori error estimators, but especially the fast identification of the periodic limits.

Abstracts of contributed talks – Session 1

New geometric approaches in solving eigenvalue problems

Foivos Alimisis, University of Geneva

We discuss recent advances on the geodesic convexity characterisation of the simple symmetric eigenvalue problem on the Grassmann manifold and analyse steepest descent type algorithms for solving it. We also show how this theory can yield to state of the art results for solving generalized eigenvalue problems. Our algorithms are competitive despite the plethora of solvers in the numerical linear algebra community and show that the theory of optimization on Riemannian manifolds can be a new wave to surf in the area. The main results we discuss are contained in https://arxiv.org/pdf/2209.03480.pdf and in ongoing works with P-A Absil, Y. Saad, B. Vandereycken and S. Vary.

Learning graph Laplacian matrices via maximum likelihood

Dimosthenis Pasadakis, USI

This talk addresses the problem of learning large graphs using an l1-regularized Gaussian maximum likelihood approach. We introduce two algorithms for the retrieval of the M-matrices that represent these graphs, that can be subsequently used for the estimation of graph Laplacians. In the first one we propose an unconstrained strategy that is based on consecutive precision matrix estimations, and in the second one we follow a constrained approach based on sequential quadratic programming. Our numerical examples and comparative results with modern open-source packages reveal that the proposed methods can accelerate the learning of graphs by up to 3 orders of magnitude, while accurately retrieving the latent graphical structure of the data. Furthermore, we conduct large scale case studies for the clustering of COVID-19 daily cases and the classification of image datasets to highlight the applicability in real-world scenarios.

Edge modes in subwavelength resonators in one dimension

Silvio Barandun, ETHZ

We present the mathematical theory of one-dimensional infinitely periodic chains of subwavelength resonators. We analyse both Hermitian and non-Hermitian systems. Subwavelength resonances and associated modes can be accurately predicted by a finite dimensional eigenvalue problem involving a capacitance matrix, which we derive from an asymptotic expansion.

The pressure-wired Stokes element: An inf-sup stable generalization of the Scott-Vogelius element

Nis-Erik Bohne, UZH

The Scott-Vogelius element (SV) $(\mathbf{S}_{k,0}(\mathscr{T}), \mathrm{div}(\mathbf{S}_{k,0}(\mathscr{T})))$ is a popular way of approximating the two-dimensional stationary Stokes equation in variational formulation. However it suffers from two major drawbacks: a) the discrete inf-sup constant deteriorates if the mesh contains *nearly* critical mesh configurations and also if the polynomial degree k is chosen to be large. b) the implementation of the condition “is a mesh point critical” is not possible and therefore replaced by a threshold condition. In order to mitigate all of these concerns we propose a parameter depending generalization of the standard SV element that replaces the threshold condition with a parameter $\eta \geq 0$ and we prove that this new element is inf-sup stable with a inf-sup constant that can be bounded from below by a constant that only depends on the shape regularity of $\mathscr{T}$, the domain and the control parameter η. These improvements come at a cost though, namely that the approximation of the velocity field $\mathbf{u}_\mathbf{S}$ in the pressure-wired Stokes element is in general not pointwise divergent free unlike the original SV element. We where able to prove that the L^2 norm of the divergence of $\mathbf{u}_\mathbf{S}$ depends at most linearly on the control parameter η and we present some numerical experiments, underlining these theoretical results.

This presentation covers joint work with B. Gräßle and S. A. Sauter

Semi-Lagrangian Finite Element Exterior Calculus for Incompressible flows

Wouter Tonnon, ETHZ

We develop a mesh-based semi-Lagrangian discretization of the time-dependent incompressible Navier-Stokes equations with free boundary conditions recast as a non-linear transport problem for a momentum 1-form. A linearly implicit fully discrete version of the scheme enjoys excellent stability properties in the vanishing viscosity limit and is applicable to inviscid incompressible Euler flows. Conservation of energy is enforced separately.

Towards finite element exterior calculus on manifolds

Martin Licht, EPFL

We discuss numerical methods for the Hodge-Laplace equation on manifolds, using the framework of finite element exterior calculus. The central tools are (i) stable commuting finite element projections and (ii) a broken Bramble-Hilbert lemma. Revisiting a classical construction by de Rham, the smoothed projection is composed of local mollification operators. The projection maps onto intrinsic finite element spaces over the manifold that are defined with respect to a smooth triangulation. The broken Bramble-Hilbert lemma follows from generalized Scott-Zhang and Clement interpolants for vector fields. Finally, if an external parametric triangulation is used, we discuss how to bound the geometric error due to variational crime. This is analogous to the convergence analysis of surface finite element methods. Our target applications include numerical relativity.

Reduced order models for time-dependent problems using the Laplace transform

Ricardo Reyes, EPFL

We propose a new method to incorporate temporal evolution into general reduced-order parametrized models. Instead of following the traditional approach of time step sampling, we use frequency-domain solutions as the data input.

In the offline stage, we transfer the problem from the time domain to the frequency domain using the Laplace transform. Then, we sample solutions for a discrete set of frequencies and use the singular valued decomposition to construct a reduced basis. And in the online part, we use the obtained reduced basis in the time-dependent problem, as we would normally do with a basis obtained with any parametric or time-sampled reduced basis method.

Although the method can be seen as a proper orthogonal decomposition extended to the frequency domain, there are two important considerations: we have to select appropriate sampling points so all the needed frequencies are captured, and we construct the basis using only the real part of the complex-valued solutions.

We present some of the harmonic analysis needed to explain the method and a two simple examples.

Overcoming the order barrier two in splitting methods when applied to semilinear parabolic problems with non-periodic boundary conditions

Ramona Häberli, University of Geneva

In general, high order splitting methods suffer from an order reduction phenomena when applied to the time integration of partial differential equations with non-periodic boundary conditions. In this talk, inspired by recent corrector techniques for the order two Strang splitting method, we introduce a splitting method of order three for a class of semilinear parabolic problems that avoids such an order reduction in the context of more general boundary conditions.

Abstracts of contributed talks – Session 2

Machine learning enhanced real-time aerodynamic forces prediction based on sparse pressure sensor inputs

Junming Duan, EPFL

Accurate prediction of aerodynamic forces in real-time is crucial for autonomous navigation of unmanned aerial vehicles (UAVs). This paper presents a machine learning-enhanced aerodynamic force prediction model based on a small number of pressure sensors located on the surface of UAV. The model is built on a linear term that can make a roughly accurate prediction and a nonlinear correction term for accuracy improvement. The linear term is based on a reduced basis reconstruction of the surface pressure distribution, in which the basis is extracted from numerical simulation data and the basis coefficients are determined by solving linear pressure reconstruction equations at a set of sensor locations. Sensor placement is optimized using the discrete empirical interpolation method (DEIM). Aerodynamic forces are computed by integrating the reconstructed surface pressure distribution. The nonlinear term is an artificial neural network (NN) that is trained to bridge the gap between ground truth and the DEIM prediction, especially in the scenario that the DEIM model is constructed based on simulation data with limited fidelity. A large network is not necessary for accurate correction as the linear model already captures the main dynamics of the surface pressure field, thus yielding an efficient DEIM+NN aerodynamic force prediction model. The model is tested on numerical and experimental dynamic stall data of a 2D NACA0015 airfoil, and numerical simulation data of the dynamic stall of a 3D drone. Numerical results demonstrate that the machine learning-enhanced model can make fast and accurate predictions of aerodynamic forces using few pressure sensors, even for the NACA0015 case in which the simulations cannot agree very well with the wind tunnel experiments, and the model is robust to noise.

Weak physics-informed neural networks for approximating entropy solutions of hyperbolic conservation laws

Tim De Ryck, ETHZ

Physics informed neural networks (PINNs) require regularity of solutions of the underlying PDE to guarantee accurate approximation. Consequently, they may fail at approximating discontinuous solutions of PDEs such as nonlinear hyperbolic equations. To ameliorate this, we propose a novel variant of PINNs, termed as weak PINNs (wPINNs) for accurate approximation of entropy solutions of scalar conservation laws. wPINNs are based on approximating the solution of a min-max optimization problem for a residual, defined in terms of Kruzkhov entropies, to determine parameters for the neural networks approximating the entropy solution as well as test functions. We prove rigorous bounds on the error incurred by wPINNs and illustrate their performance through numerical experiments to demonstrate that wPINNs can approximate entropy solutions accurately.

Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling

Eugen Bronasco, University of Geneva

B-series and generalizations are a powerful tool for the analysis of numerical integrators. An extension named exotic aromatic B-series was introduced to study the order conditions for sampling the invariant measure of ergodic SDEs. In this talk, we analyze the algebraic structures related to exotic B-series and S-series by studying the related combinatorial objects called exotic forests. We describe a theoretical algorithm that generates order conditions with respect to invariant measure and apply an algebraic framework to present a multiplicative property that ensures some order conditions to be satisfied automatically.

Spatio-Temporal Bayesian Modeling at Scale

Lisa Gaedke-Merzäuser, USI

Despite the ongoing advancements in Bayesian computing, large-scale inference tasks continue to pose a computational challenge that often requires a trade-off between accuracy and computation time. Combining solution strategies from the field of high-performance computing with state-of-the-art statistical learning techniques, we present a highly scalable approach for performing spatio-temporal Bayesian modelling based on the methodology of integrated nested Laplace approximations (INLA). The spatio-temporal model component is reformulated as the solution to a discretized stochastic partial differential equation which induces sparse matrix representations for increased computational efficiency. We leverage the power of today's distributed compute architectures by introducing a multi-level parallelism scheme throughout the algorithm. Moreover, we rethink the computational kernel operations and derive GPU-accelerated linear algebra solvers for fast and reliable model predictions.

Constructive deep neural network approximations of weighted analytic solutions to partial differential equations in polygons

Joost Opschoor, ETHZ

We construct stable, exponentially converging neural network approximations of weighted analytic functions on polygons. These appear as solutions to elliptic partial differential equations with analytic coefficient functions, right-hand side and boundary data, for example diffusion-advection-reaction equations, corresponding eigenvalue problems, linear elasticity, stationary Stokes and stationary, incompressible Navier Stokes equations. These neural networks depend on the weighted analytic function only through its values in finitely many a priori known points, whose number grows at most polylogarithmically with the desired accuracy.

Compression of Boundary Integral Operators Discretised by Anisotropic Wavelet Bases

Remo von Rickenbach, Universität Basel

Consider a domain $\Omega \subset \mathbb{R}^3$ with a Lipschitz boundary $\Gamma = \partial\Omega$. It is well-known that the Laplace problem with homogeneous Dirichlet data can be written as a boundary integral equation involving a nonlocal operator. Consequently, the resulting Galerkin matrix is densely populated.

By discretising the boundary integral equation with standard, isotropic wavelet functions, the Galerkin matrix can be compressed such that it contains only $\mathcal{O}(N)$ entries in total. The solution with respect to the compressed matrix still converges at discretisation error accuracy. Moreover, there exist respective adaptive wavelet methods, which approximate the unknown solution at the rate of the best N-term approximation with linear complexity.

However, when the boundary contains geometric, anisotropic singularities, the rate of the best N-term approximation with respect to an isotropic wavelet basis deteriorates. This obstruction might be overcome with the help of anisotropic tensor product wavelets. In this talk, we show that, in the nonadaptive case, the same properties as for the isotropic basis hold. Investigating the adaptive method is work in progress.