Scientific Committee for NUMDIFF–16

- Martin Arnold (Halle)
- Elena Celledoni (Trondheim)
- Jason Frank (Utrecht)
- Maren Hantke (Halle)
- Raphael Kruse (Halle)
- Jens Lang (Darmstadt)
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Conference office

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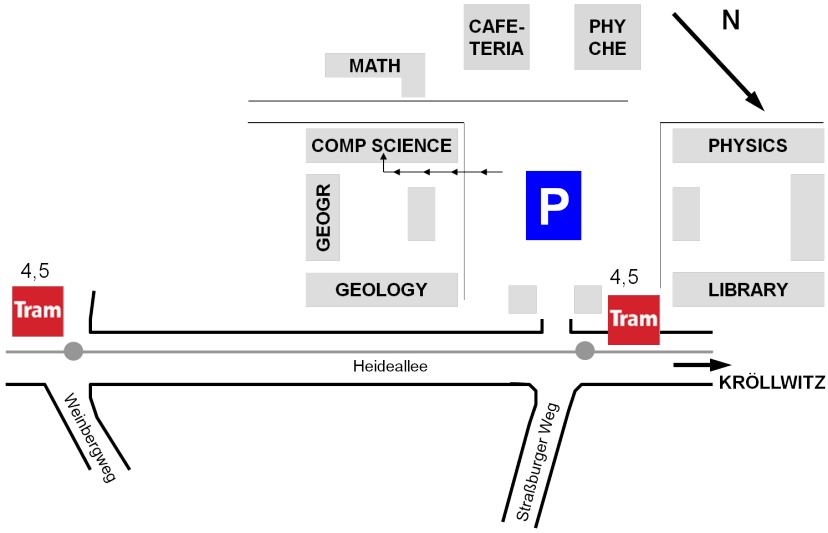
last change: 19th August 2021

Contents

1 Introduction

1. **Conference Site**
   The conference will take place in the *Computer Science building* situated within the Heide Campus at Von-Seckendorff-Platz 1. From the stop "Zentrum Neustadt" next to the "TRYP by Wyndham Halle" you can use any tram leaving eastwards, change at "Rennbahnkreuz" to tram 4 or tram 5 direction "Kröllwitz", and get off at stop "Straßburger Weg".



2. **Time Zone** The time zone for all times and dates in this programme is the Central European Summer Time (CEST = UTC+2) zone.

3. **Conference Office and Registration**
   The conference office will be open on Sunday, 5 September 2021, from 17:00 to 20:00 in the lobby of the "TRYP by Wyndham Halle" (+49 345 69310). During the week it will be situated at the conference site in room 1.03. It will be open on Monday, Tuesday and Thursday from 8:00 to 16:00, and on Wednesday and Friday from 8:00 to 12:00. You can reach the conference office by phone +49 345 5524799 (active from Monday on). Participants who have not yet paid the conference fee can pay the conference fee in cash at the conference office. Please note that we cannot accept credit cards or cheques.

4. **Lectures**
   The lecture times as given in the programme already include five minutes for discussion. Session chairs will make sure that speakers do not exceed their allocated time. All lecture rooms will be equipped with laptop and data projector.

5. **Video Streams**
   The following Zoom meeting IDs will be used:

   - Zoom Z1: Meeting ID 846 3458 1770
   - Zoom Z2: Meeting ID 939 8893 0333
   - Zoom Z3: Meeting ID 950 7034 7612

   The passcode is 162021 in all cases.

6. **Notation and hyperlinks in this document**
   An '@' symbol after a person's name indicates that this person is a remote participant.

   Z1, Z2 and Z3 indicate the Zoom meeting IDs used throughout the week.

   A hyperlink attached to a speaker's name takes you to the abstract and a hyperlink attached to a time takes you to the programme overview.

7. **Inside Numdiff**
   The protected area "Inside Numdiff" on the website is found at
   https://sim.mathematik.uni-halle.de/numdiff/Numdiff16/inside/
   and can be accessed with the login "numdiff" with password "conference2021".

   Under "Inside Numdiff" you find the Zoom links, recorded talks, slides, photos and other material which should be accessible to all participants but not to the rest of the world. It provides also a virtual noticeboard for announcements from participants to participants (e.g. other conferences, new books, open positions etc.).

8. **Coffee and Tea Breaks, Lunch**
   Coffee and tea will be provided during the morning and afternoon breaks in a room close to the conference office. For lunch, the *Mensa Weinberg* is a 15 minute walk away.

9. **Computer and Internet Access**
   At the conference site you can access the internet using eduroam or using wifi with SSID *event-net* user name *numdiff@uni-halle.de* password *up3XwFbm*. You may need to add a security exception in order to connect to this network.

10. **Conference Dinner**
    The conference dinner will be held on Thursday, at 19:00 in the "Hallesches Brauhaus", Große Nikolaistraße 2, that is in walking distance from the Tram stop Marktplatz. The dinner ticket is included in the conference fee.

11. **Tour to Naumburg Cathedral, UNESCO World Heritage**
    On Wednesday, there will be an excursion to the picturesque town Naumburg with its 750 years old cathedral that has become part of the UNESCO World Heritage in 2018. The German philosopher Friedrich Nietzsche spent his childhood and his later years in Naumburg in the home of his mother's family. The house, known as the Nietzsche-Haus, is now a museum. The Wenzelkirche hosts an impressive organ and – depending on the pandemic situation – there may be the option to climb its tower that offers a perfect view on the city of Naumburg and its surroundings.

    Buses will leave from the conference site at 12:45 and will return to Halle at around 19:30. We have guided tours through the cathedral and the treasures (on 14:30 or 16:00) and you will have time at your own disposal to explore the city center or just to have coffee and cake in one of the surrounding cafés.

12. **Conference Proceedings**
    The proceedings of NUMDIFF-16 will be published as a special issue of the Journal of Computational and Applied Mathematics. Guest editors are the members of the scientific committee and the managing guest editor is Jens Lang. Every speaker of NUMDIFF-16 can submit a manuscript for consideration of publication in this special issue. The deadline for manuscript submission is 22 January 2022. See https://sim.mathematik.uni-halle.de/numdiff/Numdiff16/proceedings.

2 Sessions

Monday

R 3.07, R 3.28 @ Z1

08:45–09:00 Opening

09:00–09:50 Michael **Dumbser**: *On structure-preserving schemes for continuum mechanics*

Coffee break

R 3.07, R 3.28 @ Z1

10:50–11:40 Gabriel **Lord**: *Adaptive timestepping for S(P)DEs.*

11:40–12:30 Chris **Budd** @: *Optimal transport methods for mesh generation in non-convex domains*

Lunch break

R 3.07 Z1

14:00–14:25 Jens **Lang**: *Super-Convergent IMEX-Peer Methods with Variable Time Steps*

14:25–14:50 Seyyed Ahmad **Hosseini**: *Efficient methods for Volterra integro-differential equations based on Floater-Hormann interpolants*

14:50–15:15 Ali **Abdi**: *Variable stepsize second derivative general linear methods*

15:15–15:40 Franco **Zivcovich**: *BAMPHI (Backward-accurate Action of Matrix PHI-functions)*

R 3.28 Z2

14:00–14:25 Caren **Tischendorf**: *Convergence Criteria for Co-Simulation of Coupled Network DAEs*

14:25–14:50 Urs **Baumgart**: *Modern Approaches and Strategies for Optimal Traffic Control*

14:50–15:15 Henning **Sauter**: *Optimal control of gas network DAEs*

15:15–15:40 Héléna **Shourick**: *Convergence acceleration of heterogeneous domain decomposition method for EMT-TS electrical network DAE system.*

R 1.23 Z3

14:00–14:25 Philipp **Reiter**: *The geometry of embeddings*

14:25–14:50 Benjamin **Bauer**: *Numerical Treatment for an Isogeometric One-Dimensional Model for Developable Flexible Elastic Strips*

14:50–15:15 Saray **Busto**: *On thermodynamically compatible schemes for turbulent shallow water flows*

15:15–15:40 Tareq **Hamadneh**: *Numerical Affine Lower Bound for Polynomials over Simplices with Applications*

Coffee break

Monday (continued)

R 3.07 Z1

16:40–17:05 Gholam Reza **Hojjati** @: *On the construction of numerical integrators for ODEs based on the linear barycentric rational interpolants*

17:05–17:30 Damien **Tromeur-Dervout**: *Schwarz and Schur time domain decomposition for nonlinear ODE*

17:30–17:55 Yohan **Eguillon**: *MISSILES: an Efficient Resolution of the Co-simulation Coupling Constraint on Nearly Linear Differential Systems through a Global Linear Formulation*

17:55–18:20 Laurent **Francois**: *High-order adaptive loose coupling of semi-discretised PDEs connected through interfacial conditions*

R 3.28 Z2

16:40–17:05 Dennis **Groh**: *Error analysis for Galerkin-BDF discretizations of nonlinear differential-algebraic systems of index-1 with an elliptic operator constraint*

17:05–17:30 Martin **Arnold**: *Multistep DAE integrators on Lie groups*

17:30–17:55 Roswitha **März**: *Overdetermined least-squares collocation for higher-index differential-algebraic equations*

R 1.23 Z3

16:40–17:05 Yvonne **Alama Bronsard**: *A new class of semi-discrete schemes for solving the Gross-Pitaevskii equation at low regularity*

17:05–17:30 Roland **Pulch**: *Methods for analysing patterns in solutions of reaction-diffusion equations*

17:30–17:55 Severiano **Gonzalez Pinto**: *High order PDE-convergence of AMF-W methods for parabolic problems*

Get Together (18:30 at Café Einstein)

Tuesday

R 3.07, R 3.28 @ Z1

08:10–09:00 Gianluigi **Rozza**: *Reduced order methods: state of the art, perspectives and applications in computational fluid dynamics*

09:00–09:50 Brynjulf **Owren**: *Deep learning as optimal control problems with applications to mechanical systems*

Coffee break

R 3.07 Z1

10:50–11:15 Paul Andries **Zegeling**: *A generalized midpoint-based boundary-value method for unstable PDEs*

11:15–11:40 Georg **Maierhofer**: *Convergence analysis of least-squares oversampled collocation for boundary element methods*

11:40–12:05 Christian **Offen**: *Turning an analysis technique into a tool: Identification and simulation of Hamiltonian systems using inverse modified equations*

R 3.28 Z2

10:50–11:15 Pedro **Lima**: *Stochastic two-dimensional neural field equation: numerical approximation and applications to working memory*

11:15–11:40 Johanna **Weinberger**: *Implicit Euler Scheme for Stochastic Partial Differential Equations with Monotone Drift*

11:40–12:05 Maria **Cabrera Calvo**: *Uniformly accurate low regularity approximations for the Klein-Gordon equation and Klein-Gordon-Schrödinger systems*

R 1.23 Z3

10:50–11:00 Leonardo **Colombo** @: *Geometric integration for the formation control of multi-agent systems*

11:00–11:10 David **Martin de Diego** @: *Geometric nonholonomic integrators*

11:10–11:20 Elena **Chistyakova** @: *Some Properties of Higher Order Differential Algebraic Equations with Singular Points*

11:20–11:30 Charlélie **Bertrand** @: *Numerical Dynamics of a Cable Subjected to Frictional Impact*

11:30–11:40 Zoltán **Horváth** @: *A novel POD-DEIM-like model reduction method for the compressible Euler and Navier-Stokes equations*

11:40–11:50 Neisser **Pino Romero** @: *A Computational Model of Dengue Transmission by Cellular Automata*

Lunch break

Tuesday (continued)

Minisymposium "ODE and SDE methods in machine learning"

organised by Ben Leimkuhler

R 3.07 Z1

13:30–14:00 Siddhartha **Mishra** @: *Recurrent Neural Networks inspired by ODEs*
14:00–14:30 Lu **Lu** @: *Learning nonlinear operators via DeepONet*
14:30–15:00 Han **Wang** @: *Modeling the interatomic potential by deep learning*
15:00–15:30 Matt **Graham** @: *Lift and flow: manifold MCMC methods for efficient inference in stiff posteriors*

Coffee break

R 3.07 Z1

16:30–17:00 Zhen **Zhang** @: *SympNets & PNNs: Intrinsic structure-preserving networks for identifying Hamiltonian & Poisson systems*
17:00–17:30 Adrià **Garriga-Alonso** @: *Training neural networks with corrected Langevin dynamics and stochastic gradients*
17:30–18:00 Tiffany **Vlaar** @: *Multirate Training of Neural Networks*
18:00–18:30 Thomas **Richter** @: *A posteriori error estimation for Physics Inspired Neural Network solutions to partial differential equations*

Minisymposium "Numerical methods in fractional calculus"

organised by Roberto Garrappa

R 3.28 Z2

13:30–14:10 Łukasz **Płociniczak**: *Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology*
14:10–14:50 Marina **Popolizio**: *On the efficient numerical computation of the matrix Mittag-Leffler function*
14:50–15:30 Roberto **Garrappa**: *A change of perspective in variable-order fractional calculus*

Coffee break

R 3.28 Z2

16:30–17:10 Natalia **Kopteva** @: *Pointwise-in-time a posteriori error control for time-fractional parabolic equations*
17:10–17:50 Angelamaria **Cardone** @: *A class of spectral methods for deterministic and stochastic fractional differential equations.*
17:50–18:30 Eva **Kaslik** @: *Stability analysis of multi-order fractional differential equations*

Minisymposium "THREAD - Interactions of beam like structures"

organised by Narges Mohammadi, Konstantina Ntarladima, Jan Tomec, and Gordan Jelenić

R 1.23 Z3

13:30–14:00 Seevani **Bali** @: *Implementation of geometrically-exact beam theory using finite volume discretisation and its analogy to the finite element approach*

14:00–14:30 Juliano **Todesco**: *On the exact tangent matrices of a geometrically exact beam formulated on the special Euclidean group SE(3)*

14:30–15:00 Toni **Jelusic** @: *Geometrically exact beam theory - Implementation based on automatic differentiation with the AceGen/AceFEM system*

15:00–15:30 Jonas **Harsch**: *Spatial nonlinear beam theory for soft pneumatic actuators*

Coffee break

R 1.23 Z3

16:30–17:00 Mohammad Ali **Saadat** @: *Investigation of the role of frictional contact interactions in the mechanical response of spiral strands using 1D finite strain beam model*

17:00–17:30 Davide **Manfredo**: *Modeling of inelastic effects in composite cables by means of Hysteresis operators*

17:30–18:00 Marielle **Debeurre** @: *Efficient nonlinear modeling of highly flexible beam structures using geometrically exact beam models*

18:00–18:30 Sudhanva **Kusuma Chandrashekhara** @: *Computational aspects of the velocity based elements in post-buckling analysis of beams and frames.*

Wednesday

R 3.07, R 3.28 @ Z1

08:00–08:10 John **Butcher** @: *Isomeric trees with applications to Runge-Kutta methods*

R 3.07, R 3.28 @ Z1

08:10–09:00 Klas **Modin** @: *Long-time simulation of spherical hydrodynamics via quantization*

09:00–09:50 Sebastiano **Boscarino** @: *Implicit-explicit (IMEX) methods for evolutionary partial differential equations*

Coffee break

R 3.07 Z1

10:50–11:00 Gianluca **Frasca-Caccia** @: *Exponentially Fitted Methods that Preserve Conservation Laws*

11:00–11:10 Piotr **Skrzypacz** @: *Numerical simulations of dead zone formation in the catalytic flow-through membrane reactor*

11:10–11:20 Christoph **Zimmer** @: *Bulk-surface Lie splitting for parabolic problems with dynamic boundary conditions*

11:20–11:30 Gobinda **Garai** @: *Convergence of the Neumann-Neumann Method for the Cahn-Hilliard Equation*

R 3.28 Z2

10:50–11:00 Carmela **Scalone** @: *Numerical modeling for stochastic oscillators*

11:00–11:10 Giuseppe **Giordano** @: *Continuous-time extensions of stochastic one-step methods*

11:10–11:20 Monika **Eisenmann** @: *Sub-linear convergence of a tamed stochastic optimization method*

11:20–11:30 Måns **Williamson** @: *SRKCD: a stabilized Runge-Kutta method for large-scale optimization problems*

11:30–11:40 Helmut **Podhaisky**: *On randomized implicit Runge–Kutta methods*

R 1.23 Z3

10:50–11:00 Giovanni **Pagano** @: *Adapted numerical schemes for differential problems*

11:00–11:10 Leila **Moradi** @: *Frequency evaluation for adapted peer methods*

11:10–11:20 Omar **Khalil** @: *Approximation of Functions and Solutions to Ordinary Differential Equations by Adaptive Poly-Sinc Methods*

11:20–11:30 Yagub **Aliyev** @: *Numerical solutions of Sturm-Liouville problems with a boundary condition depending on an eigenparameter*

11:30–11:40 Mufutau **Rufai** @: *A pair of two-step hybrid block methods using a variable stepsize formulation for integrating third-order Lane-Emden-Fowler equations.*

Lunch break

Thursday

R 3.07, R 3.28 @ Z1

08:10–09:00 Katharina **Schratz**: *Resonances as a computational tool*

09:00–09:50 Ulrik Skre **Fjordholm** @: *Numerical methods for conservation laws on graphs*

Coffee break

R 3.07, R 3.28 @ Z1

10:50–11:40 Sina **Ober-Blöbaum**: *Variational Integrators: high order, multirate dynamics and optimal control*

Lunch break

Minisymposium "Fluid dynamics: Innovative discretisations and algorithms"

organised by Colin Cotter

R 3.07 Z1

13:00–13:30 Lawrence **Mitchell**: *Augmented Lagrangian preconditioning for fluids: theory and practice*

13:30–14:00 Jemma **Shipton**: *Compatible finite elements and parallel-in-time schemes for geophysical fluid dynamics*

14:00–14:30 Gabriel R. **Barrenechea** @: *Divergence-free finite element methods for an inviscid fluid model*

14:30–15:00 Tomasz **Tyranowski**: *Stochastic variational principles for the collisional Vlasov-Maxwell and Vlasov-Poisson equations*

Coffee break

R 3.07 Z1

16:00–16:30 Werner **Bauer** @: *Higher order phase averaging for highly oscillatory systems*

16:30–17:00 Artur **Palha** @: *Dual field mass-, energy-, and helicity conserving discretization for the incompressible Navier-Stokes equations*

17:00–17:30 Martin **Schreiber** @: *Cauchy Contour Integration based REXI methods for Climate and Weather simulations*

17:30–18:00 Yu-hsuan **Shih** @: *Advanced Newton methods for geodynamical models of Stokes flow with viscoplastic rheologies*

Thursday (continued)

Minisymposium "Numerical methods for stochastic evolution equations"

organised by Raphael Kruse

R 3.28 Z2

13:00–13:30 Annika **Lang** @: *Connecting random fields on manifolds and stochastic partial differential equations in simulations*

13:30–14:00 Andreas **Petersson** @: *Approximation of SPDE covariance operators by finite elements: A semigroup approach*

14:00–14:30 Andreas **Rößler** @: *Numerical simulation of stochastic evolution equations with non-commutative noise*

14:30–15:00 Julian **Clausnitzer** @: *Numerical Solution of two-dimensional parabolic SPDEs using a Galerkin exponential time differencing scheme combined with a boundary integral formulation*

Coffee break

R 3.28 Z2

16:00–16:30 Maximilian **Schade**: *Monotone SPDEs with Algebraic Constraints*

16:30–17:00 Rico **Weiske**: *The BDF2-Maruyama Method for Stochastic Evolution Equations with Monotone Non-Lipschitz Drift*

17:00–17:30 Erika **Hausenblas** @: *Systems with Stochastic Pattern Formation*

17:30–18:00 David **Cohen** @: *Time integration of the stochastic Manakov equation*

Minisymposium "THREAD - Geometric numerical integration"

organised by Andrea Leone, Ergys Çokaj, Martina Stavole, and Sigrid Leyendecker

R 1.23 Z3

13:00–13:30 Denise **Tumiotto**: *Numerical investigation of stability of coarse grid discretisations for dissipative systems*

13:30–14:00 Emina **Hadzialic**: *Modelling and Simulation of the Convection-Diffusion Equation through Fractional Restricted Calculus of Variations*

14:00–14:30 Yana **Lishkova**: *A multirate variational approach to simulation and optimal control for flexible spacecraft*

14:30–15:00 Rodrigo T. **Sato Martín de Almagro**: *High-order integrators on homogeneous spaces via nonholonomic mechanics*

Coffee break

R 1.23 Z3

16:00–16:30 Armin **Bosten**: *The SE(3) Lie group framework for flexible multibody systems with contact*

16:30–17:00 Davide **Murari**: *Learning the Hamiltonian of some classes of mechanical systems*

17:00–17:30 Stefano **Di Giovacchino**: *Long-term analysis of stochastic Hamiltonian systems under time discretizations*

Conference Dinner (19:00 at ???)

Friday

R 3.07, R 3.28 @ Z1

08:10–09:00 Dajana **Conte** @: *Recent advances in deterministic and stochastic numerics for evolutive problems*

09:00–09:50 Gilles **Vilmart**: *Superconvergent methods inspired by the Crank-Nicolson scheme in the context of diffusion PDEs (deterministic and stochastic)*

Coffee break

R 3.07, R 3.28 @ Z1

10:50–11:40 Maren **Hantke**: *Discretization of a phase field model*

11:40–12:30 Ari **Stern**: *Structure-preserving hybrid methods*

12:30–12:40 Closing

3 Abstracts

Variable stepsize second derivative general linear methods
Ali Abdi (University of Tabriz), Arash Jalilian, Gholamreza Hojjati
Mon 14:50-15:15 R3.07 Z1

Implementation of second derivative general linear methods (SGLMs) using the Nordsieck technique have been already studied and an efficient MATLAB code based on an L–stable SGLM of order four has been developed in a variable stepsize environment. This talk is about variable stepsize SGLMs which provides an alternative to the Nordsieck technique of changing the stepsize of integration. This approach is based on the derivation of the methods based directly on nonuniform grid so that the coefficients matrices of the methods depend, in general, on the ratios of the current stepsize and the past stepsizes. For such methods, it is not required to update the input vector for the new stepsize; actually, the output vector of the last step can be directly used in the next step as the input vector.
Keywords: Ordinary differential equations, General linear methods, Second derivative methods, Variable stepsize, Order conditions.

A new class of semi-discrete schemes for solving the Gross-Pitaevskii equation at low regularity
Yvonne Alama Bronsard (Sorbonne Université), Katharina Schratz
Mon 16:40-17:05 R1.23 Z3

In this talk I will introduce a novel time discretization for the Gross-Pitaevskii equation at low-regularity on an arbitrary domain $\Omega \subset \mathbb{R}^d$, $d \leq 3$, with non-smooth potential. I will first show the construction of our first and second order low-regularity integrators. I will discuss the stability issues which arise during the construction of the second-order low-regularity integrator, and will then propose two different approaches to guarantee the stability of our proposed scheme.
I will also present a local and global $L^2(\Omega)$ and $H^1(\Omega)$ error analysis for the first and second low-regularity integrators, and for a class of solutions and potential in appropriate Sobolev spaces.
These new schemes, together with their optimal local error, allow for convergence under lower regularity assumptions than required by classical methods.

Numerical solutions of Sturm-Liouville problems with a boundary condition depending on an eigenparameter
Yagub Aliyev (ADA University)
Wed 11:20-11:30 R1.23 Z3

The following spectral problem is considered

$$-y'' + q(x)y = \lambda y,\ 0 < x < 1, \tag{1}$$

$$y(0)\cos\beta = y'(0)\sin\beta,\ 0 \leq \beta < \pi, \tag{2}$$

$$y(1) = (c\lambda + d)y'(1), \tag{3}$$

where c, d are real constants and $c > 0$, λ is the spectral parameter, $q(x)$ is a real valued and continuous function over the interval $[0, 1]$.

In the current study we are mainly interested in numerical evaluation of the eigenvalues and the eigenfunctions of special eigenvalue problems such as

$$-y'' = \lambda y,\ 0 < x < 1,$$

$$y(0) = 0,$$

$$y(1) = \left(\frac{\lambda}{3} + 1\right) y'(1).$$

For this problem $\lambda_0 = \lambda_1 = 0$ is a double eigenvalue.The other eigenvalues $\lambda_2 < \lambda_3 < \dots$ are the solutions of the equation $\tan\sqrt{\lambda} = \sqrt{\lambda}\left(\frac{\lambda}{3} + 1\right)$. Eigenfunctions are $y_0 = x$, $y_n = \sin\sqrt{\lambda_n}x$ $(n \geq 2)$ and an associated function corresponding to y_0 is $y_1 = -\frac{1}{6}x^3 + Cx$, where C is an arbitrary constant. The transcendental equation $\tan\sqrt{\lambda} = \sqrt{\lambda}\left(\frac{\lambda}{3} + 1\right)$ is approximately solved to find approximate values of λ_n which then used to find formula for $y_n = \sin\sqrt{\lambda_n}x$.
We also discuss an example for which the eigenvalue is triple.

Multistep DAE integrators on Lie groups

Martin Arnold (Martin Luther University Halle-Wittenberg), Victoria Wieloch, Stefan Hante

Mon 17:05-17:30 R3.28 Z2

We consider the time discretization of differential equations on Lie groups by a class of multistep methods that define the solution updates in each time step by the exponential of solution increments in the corresponding Lie algebra. An increment representation of classical multistep methods proves to be favourable to define a Lie group specific correction term for updating the solution increments. This correction term does not require any extra effort for methods of order $p \leq 2$. Up to order $p = 4$, there is just one commutator to be evaluated in each time step which makes this approach more efficient than other multistep integrators for ODEs on Lie groups.
Our main interest is in the application to constrained systems on Lie groups. We discuss zero stability and convergence in the application to DAEs of index 2 and 3. The results of the theoretical investigations are verified by numerical tests for a benchmark problem and by a comparison with other Lie group integrators in the application to a semi-discretized rod model from nonlinear beam theory.

Implementation of geometrically-exact beam theory using finite volume discretisation and its analogy to the finite element approach

Seevani Bali (School of Mechanical and Materials Engineering, University College Dublin), Željko Tuković, Philip Cardiff, Vikram Pakrashi

Tue 13:30-14:00 R1.23 Z3

Keywords: *geometrically exact beam, finite volume method, finite rotations, large displacements, Newton-Raphson*

This study focuses on Finite-Volume (FV) discretisation of geometrically-exact beam theory and its efficacy to solve established benchmark cases. Several authors have investigated a range of geometrically nonlinear problems subjected to large displacements and rotations mostly using finite element (FE) approximations [1, 2]. Recent developments of Tuković *et al.* [3] have focused on the implementation of the geometrically-exact beam theory using the FV method to model shear-deformable circular cross-sectional beams. In this work, we use a FV solver to simulate distinct benchmark cases and provide an analogy of the FV method to the widely accepted FE approximations. The FV method is mostly popular in the field of computational fluid dynamics

and only in the past few decades, has been applied to the field of solid mechanics [4]. This paper uses a cell-centred FV approach to discretise the spatial domain of the beam model into a set of uniform control volumes (CVs) and the governing equations are balanced across all the internal faces enclosed by the CV. The nonlinear stress resultant equations of spatial forces and moments are linearised and iteratively solved for incremental displacements and incremental rotations using a Newton-Raphson procedure. For the benchmark cases, the accuracy of results obtained using the FV method is compared against the existing numerical results achieved using the FE approach. The results of the research show that the simple, yet powerful and naturally conservative FV approach can be used as an alternative to the FE approximations for such large displacement and rotation problems.

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[1] Simo, J.C., 1985. A finite strain beam formulation. The three-dimensional dynamic problem. Part I. *Computer methods in applied mechanics and engineering*, 49(1), pp.55-70.

[2] Ibrahimbegovic, A., 1997. On the choice of finite rotation parameters. *Computer Methods in Applied Mechanics and Engineering*, 149(1-4), pp.49-71.

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[4] Cardiff, P. and Demirdžić, I., 2021. Thirty years of the finite volume method for solid mechanics. *Archives of Computational Methods in Engineering*, pp.1-60.

Divergence-free finite element methods for an inviscid fluid model

Gabriel R. Barrenechea (University of Strathclyde), Naveed Ahmed, Erik Burman, Johnny Guzman, Christian Merdon, Alexander Linke

Thu 14:00-14:30 R3.07 Z1

In this talk I will review some recent results [1,2] on the stabilisation of linearised incompressible inviscid flows (or, with a very small viscosity). The partial differential equation is a linearised incompressible equation similar to Euler's equation, or Oseen's equation in the vanishing viscosity limit. In the first part of the talk I will present results on the well-posedness of the

partial differential equation itself. From a numerical methods' perspective, the common point of the two worksis the aim of proving the following type of estimate:

$$\|\boldsymbol{u} - \boldsymbol{u}_h\|_{L^2} \leq C\, h^{k+\frac{1}{2}} |\boldsymbol{u}|_{H^{k+1}}, \tag{1}$$

where $\boldsymbol{u}$ is the exact velocity and $\boldsymbol{u}_h$ is its finite element approximation. In the estimate above, the constant C is independent of the viscosity (if the problem has a viscosity), and, more importantly, independent of the pressure. This estimate mimics what has been achieved for stabilised methods for the convection-diffusion equation in the past. Nevertheless, up to the best of our knowledge, had only been achieved for Oseen's equation using equal-order elements, and assuming a (very) regular pressure.
I will first present results of a discretisation using $H(div)$-conforming spaces, such as Raviart-Thomas, or Brezzi-Douglas-Marini, where an estimate of the type (1) is proven (besides an optimal estimate for the pressure). In the second part of the talk I will move on to H^1-conforming divergence-free elements, with the Scott-Vogelius element as the prime example. In this case, dueto the H^1-conformity, the need of an extra control of the vorticity equation, and some appropriate jumps, appears. So, a new stabilised finite element method adding control on the vorticity equation is proposed. The method is independent of the pressure gradients, which makes it pressure-robust and leads to pressure-independent error estimates such as (1). Finally, some numerical results will be presented and the present approach will be compared to the classical residual-based SUPG stabilisation.

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Numerical Treatment for an Isogeometric One-Dimensional Model for Developable Flexible Elastic Strips

Benjamin Bauer (Fraunhofer Institute for Industrial Mathematics (ITWM)), Michael Roller, Joachim Linn, Bernd Simeon

Mon 14:25-14:50 R1.23 Z3

Numerous engineering applications deal with thin-walled structural parts, an example being flexible flat cables in the development of consumer electronics or computer hardware. Classical shell models describe such slender objects at hand of their centre-surface in order to reduce the involved number of degrees of freedom and thereby the numerical costs.
Several research contributions [1] within the last century continued this idea of dimensional reduction for isometric deformations of developable base surfaces. Recently, this lead to shell descriptions depending on one parameter and, therefore, resembling rod models. For example, Starostin and van der Heijden [2] based their model on the envelope of rectifying planes.
We circumvent problems arising with vanishing curvature of the centre line by utilising a relatively parallel frame [3] along the base curve. This enables us to generalise the concept of rectifying developable surfaces to curves with much softer regularity requirements.
Isometric deformations of the centre surface preserve the developabilty of a plane reference configuration. Thus, there is no membrane strain involved and the stored energy functional

consists only of the bending energy. An optimisation problem with highly non-linear geometric constraints and boundary conditions yields the equilibrium state as a local minimum.
We discuss numerical issues associated with the applied penalty formulation and isogeometric discretisation at hand of use cases for strips clamped at both ends.

References

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Higher order phase averaging for highly oscillatory systems

Werner Bauer (Imperial College London), Colin J. Cotter, Beth Wingate

Thu 16:00-16:30 R3.07 Z1

We introduce a higher order phase averaging method for nonlinear oscillatory systems. Phase averaging is a technique to filter fast motions from the dynamics whilst still accounting for their effect on the slow dynamics. Phase averaging is useful for deriving reduced models that can be solved numerically with more efficiency, since larger timesteps can be taken. Recently, Haut and Wingate (2014) introduced the idea of computing finite window numerical phase averages in parallel as the basis for a coarse propagator for a parallel-in-time algorithm. In this contribution, we provide a framework for higher order phase averages that aims to better approximate the unaveraged system whilst still filtering fast motions. Whilst the basic phase average assumes that the solution is independent of changes of phase, the higher order method expands the phase dependency in a basis which the equations are projected onto. We illustrate the properties of this method on an ODE that describes the dynamics of a swinging spring due to Lynch (2002). Although idealized, this model shows an interesting analogy to geophysical flows as it exhibits a slow dynamics that arises through the resonance between fast oscillations. On this example, we show convergence to the non-averaged (exact) solution with increasing approximation order also for finite averaging windows. At zeroth order, our method coincides with a standard phase average, but at higher order it is more accurate in the sense that solutions of the phase averaged model track the solutions of the unaveraged equations more accurately.

Modern Approaches and Strategies for Optimal Traffic Control

Urs Baumgart (Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM), Michael Burger

Mon 14:25-14:50 R3.28 Z2

An increasing amount of traffic, accompanied by traffic jams and negative environmental impacts, has led, already today, to a high demand for intelligent mobility solutions. At the same time, today's vehicle technology allows to collect an increasing amount of data to improve the vehicles' performance, reliability and safety. Concerning mobility infrastructure, larger and larger datasets can be transmitted faster every year, and new communication technology, such as 5G, is emerging and maturing permanently.
We study approaches to use (real-time) data, communicated between cars and infrastructure,

to improve and to optimize traffic flow in the future and, thereby, to support holistic, efficient and sustainable mobility solutions.
To build traffic networks of varying complexity, we consider microscopic traffic models. In these models, single cars and their longitudinal dynamics are modelled via coupled systems of ordinary differential equations (ODEs). Whereas most cars are set up to behave like human drivers, we assume that certain cars have an additional intelligent controller that obtains real-time information from other vehicles. Moreover, these controllers use a model predictive control (MPC) approach and optimal control theory with the overall goal to improve traffic flow for all vehicles in the considered system.
A leading example in this contribution is a virtual version of the prominent ring road experiment [1]. Realistic, human-like driving rapidly generates stop-and-go waves in that experiment. We show that the use of one single, intelligently controlled vehicle as described above, is able to prevent those stop-and-go situations completely. Based on this example, we analyse different optimal control methods and we study different amounts of model-knowledge for the controller as well as varying set-ups of the underlying dynamical system. We present an approach to substitute the MPC controller by a model based on machine learning techniques ("imitation learning") that mimics the MPC controller's behaviour, but requires much less computing times. Last not least, we compare these approaches with model-free *Reinforcement Learning* methods and feedback control based on neural networks.

References

[1] Sugiyama, Y., Fukui, M., Kikuchi, M., Hasebe, K., Nakayama, A., Nishinari, K., Tadaki, S.-i., and Yukawa, S. (2008). Traffic jams without bottlenecks—experimental evidence for the physical mechanism of the formation of a jam. *New Journal of Physics*, 10(3):033001.

Numerical Dynamics of a Cable Subjected to Frictional Impact

Charlélie Bertrand (Univ Lyon, ENTPE, LTDS UMR CNRS 5513), Acary Vincent , Lamarque Claude-Henri

Tue 11:20-11:30 R1.23 Z3

The dynamics of an elastic cable subjected to frictional contact are investigated numerically. The talk will address the formulation of a Finite Element formulation for the finite displacement of one cable subjected to the presence of one obstacle.

The cable is a curvilinear domain which torsion and bending are negligible compared to the axial force, termed as tension. Moreover, the cable is a structure which cannot overcome compression. The position and velocity of the centerline are given at any time t through the relation $S \to (q(S,t), v(S,t))$ where S is a curvilinear coordinate in the unstretched configuration. In the sequel, these dependencies are omitted for conciseness. We will refer to S and t differentiation with $\bullet'$ and $\dot{\bullet}$. The local form of system equations [1, 2] are given as follows:

$$\rho\dot{v} + 2cv = \left(EA\left(\|q'\| - 1\right)' \frac{q'}{\|q'\|} \right) + f \quad \text{such that } \|q'\| - 1 \geqslant 0 \tag{1}$$

It will be explained how a discrete nonlinear problem is obtained to predict the unconstrained dynamics of the cable in the following matrix form via finite element method [3] and how the latter is reformulated into a measure differential inclusion

$$\mathbf{M}\dot{\mathbf{v}} + \mathbf{C}(\mathbf{q})\mathbf{v} + \mathbf{K}(\mathbf{q})\mathbf{q} = \mathbf{f} \rightsquigarrow \begin{cases} \mathbf{M}\mathrm{d}\mathbf{v} + \mathbf{C}(\mathbf{q})\mathbf{v}\mathrm{d}t + \mathbf{K}(\mathbf{q})\mathbf{q}\mathrm{d}t = \mathbf{f}\mathrm{d}t + \mathrm{d}\mathbf{r} \\ \mathbf{v}^+ = \dot{\mathbf{q}}^+ \\ \mathbf{q}(t=0) \in \mathcal{C}(t=0)\ ,\ \mathbf{v}(t=0^-) = \dot{\mathbf{q}}_0 \end{cases} \tag{2}$$

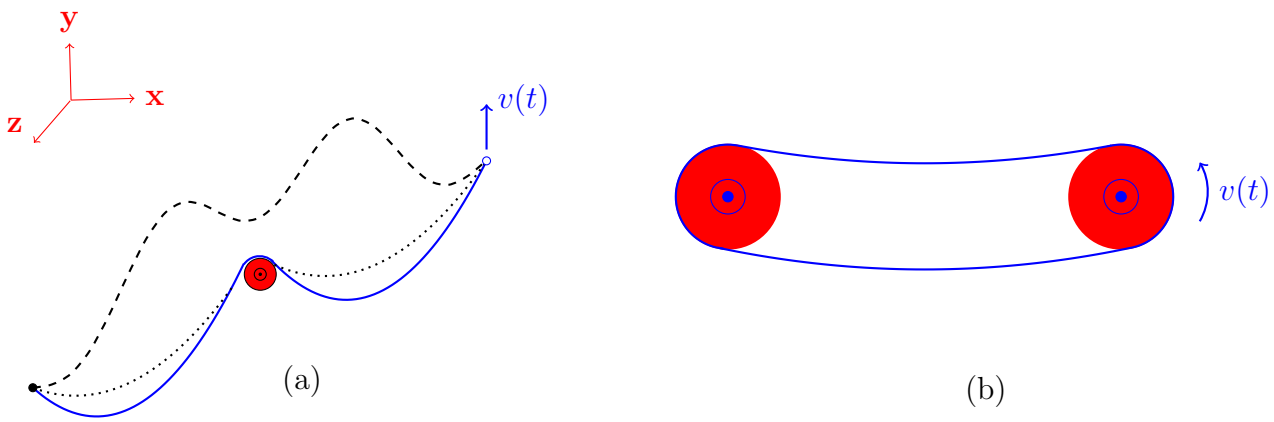

Figure 1: (a) Cable with moving end-support subjected to the presence of a circular obstacle - (b) Belt-pulley system

where $\mathcal{C}(t)$ is defined as the subspace where the dynamics are constrained to evolve, here due to the presence of one obstacle, which reads

$$\mathcal{C}(t) = \Big\{ \mathbf{q} \in \mathbb{R}^d \ , \ \mathbf{g}(\mathbf{q}) \geqslant \mathbf{0} \ \text{(vector inequality)} \Big\} \tag{3}$$

The measure differential inclusion will be used to derive a time-stepping scheme called the NonSmooth Contact Dynamics methods [4]. The latter relies on an implicit scheme of low order which can handle jumps at the velocity level. A restitution coefficient, e, links the velocity befrore and after impact and the Coulomb law is used to model the friction (μ Coulomb coefficient). At each time step, the frictional contact problem is attacked via Lemke Method [5]. It will be explained how the local coordinates at contacting points yields to solve the Linear Complementarity Problem just below

$$\left\{ \begin{array}{l} \mathbf{v}^{k+1} = \mathbf{v}^f + \widehat{\mathbf{M}}^{-1} \Big(\mathbf{H}_N^\top \mathbf{r}^1 + \mathbf{H}_T^\top \Big(\mu \mathbf{r}^1 - \mathbf{r}^2 \Big) \Big) \quad , \quad \widehat{\mathbf{M}} = \mathbf{M} + h\mathbf{C} + h^2 \Delta \mathbf{K} \\ \mathbf{u}_N^1 = \mathbf{H}_N \mathbf{v}^f \ , \ \mathbf{u}_N^0 = \mathbf{H}_N \mathbf{v}^k \ , \ \mathbf{u}_T^1 = \mathbf{H}_T \mathbf{v}^f \ , \ \mathbf{u}_T^0 = \mathbf{H}_T \mathbf{v}^k \\ \quad \text{For all } \alpha \text{ such that } \Big(\mathbf{g}(\mathbf{q}^k + h\mathbf{v}^f) \Big)_\alpha \leqslant 0 : \\ \quad \mathbf{0} \leqslant \begin{bmatrix} \widehat{\mathbf{W}}_{NN} + \mu \widehat{\mathbf{W}}_{NT} & -\widehat{\mathbf{W}}_{NT} & \mathbf{0} \\ -\widehat{\mathbf{W}}_{TN} - \mu \widehat{\mathbf{W}}_{TT} & \widehat{\mathbf{W}}_{TT} & \mathbf{I} \\ 2\mu \mathbf{I} & -\mathbf{I} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{r}_\alpha^1 \\ \mathbf{r}_\alpha^2 \\ (\mathbf{u}_T^1)^+ \end{bmatrix} + \begin{bmatrix} (\mathbf{u}_N^1)_\alpha + e\,(\mathbf{u}_N^0)_\alpha \\ -\,(\mathbf{u}_T^1)_\alpha \\ \mathbf{0} \end{bmatrix} \perp \begin{bmatrix} \mathbf{r}_\alpha^1 \\ \mathbf{r}_\alpha^2 \\ (\mathbf{u}_T^1)^+ \end{bmatrix} \geqslant \mathbf{0} \\ \quad \text{For all } \alpha \text{ such that } \Big(\mathbf{g}(\mathbf{q}^k + h\mathbf{v}^f) \Big)_\alpha > 0 : \\ \quad \mathbf{r}_\alpha^1 = \mathbf{0} \quad , \quad \mathbf{r}_\alpha^2 = \mathbf{0} \end{array} \right. \tag{4}$$

where $\mathbf{v}^f$ is the unconstrained velocity predicted by FEM and $(\mathbf{u}_T^1)^+$ is the positive part of $\mathbf{u}_T^1$. We used a modified Delassus operator given by the following expression:

$$\widehat{\mathbf{W}}_{NN} = \mathbf{H}_N \widehat{\mathbf{M}} \mathbf{H}_N \ , \ \widehat{\mathbf{W}}_{NT} = \mathbf{H}_N \widehat{\mathbf{M}} \mathbf{H}_T \ , \ \widehat{\mathbf{W}}_{TN} = \mathbf{H}_T \widehat{\mathbf{M}} \mathbf{H}_N \ , \ \widehat{\mathbf{W}}_{TT} = \mathbf{H}_T \widehat{\mathbf{M}} \mathbf{H}_T \tag{5}$$

Some applications will be presented for belt-pulley systems and for the vibration of a cable subjected to the presence of an obstacle ; Systems are depicted in Figure 1.

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Implicit-explicit (IMEX) methods for evolutionary partial differential equations

Sebastiano Boscarino (University of Catania)

Wed 09:00-09:50 R3.07, R3.28 @ Z1

Several models in science, physics and engineering, are described by evolutionary systems of partial differential equations (PDEs). A vast literature exists on space and time discretization of such systems, and it is sometimes difficult to identify which is the appropriate technique to use for a particular problem. A well-known approach in the numerical solution of evolutionary problems in PDEs is the method of lines (MOL), in which a system of PDEs is first discretized in space by some suitable technique (finite difference, finite volume, finite element or discontinuous Galerkin), thus obtaining a large system of ordinary differential equations (ODEs), and then an ODE solver is used to find the desired numerical approximation to the problem. Traditionally, most systems of ODE's are classified as stiff or non-stiff, according to the ratio between the fastest and slowest time scales involved, and, accordingly, stiff or non-stiff ODE solvers are used for their numerical solution. When dealing with PDEs, there are many stiff problems, however, in which a fully implicit treatment becomes prohibitively expensive, and several terms of the system can be treated explicitly. In such cases Implicit-Explicit (IMEX) methods represent a natural approach, maintaining the desired stability properties without the computational cost of a fully implicit method. This talk will focus on IMEX methods, with particular emphasis on their application to systems of PDEs. Indeed, IMEX have shown to be a very effective tool for the numerical solution of a wide class of evolutionary problems, in several contexts: kinetic theory of rarefied gases, linear and nonlinear waves, viscoelasticity, multiphase flows, radiation hydrodynamics, traffic flows, shallow water, just to mention some examples. Furthermore, these methods are optimal ODE solvers for some classes of ODEs such as, for example, singular perturbation problems, which are commonly found in many areas of applied mathematics, including fluid dynamics and boundary value problems containing a small parameter, stiff nonlinear oscillators, or chemical kinetics with slow and fast reactions. IMEX methods of Runge Kutta and linear multistep type have been extensively employed for evolutionary PDEs in combination with a wide range of spatial discretization. They, also provide an ideal framework for the construction of asymptotic preserving methods, currently very popular in the context of fluid-dynamical limits of kinetic equations. Nowadays, these methods have become mainstream for the solution of evolutionary PDEs, in particular in the field of hyperbolic and kinetic equations. The construction, analysis and application of IMEX methods, developed in the last two decades, will be summarized and illustrated with the help of several examples, and test cases.

The SE(3) Lie group framework for flexible multibody systems with contact

Armin Bosten (University of Liège), A. Cosimo, J. Linn, O. Brüls

Thu 16:00-16:30 R1.23 Z3

The kinematic description of multibody systems makes extensive use of the notion of frames. Frame operations may be described in a systematic manner using concepts from differential geometry and Lie groups, where a frame transformation is represented by an element of the special Euclidean group $SE(3)$. Working with left invariant derivatives and a consistent spatial discretization leads to equations of motion formulated on a Lie group. Forces, strain measures, arbitrary virtual motions and velocities are expressed in the local body-attached frame such that the equations only depend on relative motions between frames [1, 2]. Kinematic joints i.e., restricted relative motion modeled as bilateral constraints [3], can be handled conveniently. Indeed, the $SE(3)$ element that describes relative transformations is invariant under superimposed Euclidean transformation. As it will be shown in this contribution, the same can be said for contact conditions written as unilateral constraints and the associated constraint gradient. The constraints are enforced using an augmented Lagrangian approach. An implicit Lie group time integration scheme is employed [4]. The mass matrices and tangent stiffness contributions of each element required for the semismooth Newton algorithm are invariant under rigid body motions. Interestingly, during the entire formulation and discretization procedure, no global parametrization of rotation is introduced and the non-linearity of the equations is reduced as opposed to other formulations.

References

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Optimal transport methods for mesh generation in non-convex domains

Chris Budd (University of Bath), Tristan Pryer, Simone Appella

Mon 11:40-12:30 R3.07, R3.28 @ Z1

r-adaptive mesh generation by using moving meshes for the computational solution of PDEs can be done effectively by using optimal transport (OT) methods. This proves to be a robust and reliable way of generating meshes with provable regularity and skewness measures. Finding the best mesh on which to solve a PDE then becomes a problem of solving a fully nonlinear time-evolving system on an appropriate manifold with appropriate boundary conditions. The regularity of the mesh then follows from rigorous estimates of the solution of the fully nonlinear problem.

In this talk I will describe the ideas behind using OT methods for mesh generation. These involve solving Monge-Ampére equations (or Monge-Ampére like equations in the case of the sphere) of the general form

$$m(\nabla\phi)H(\phi) = \theta$$

where $m(\nabla\phi)$ is a 'monitor function' related to the solution of the underlying PDE which is constructed to be a measure of the solution error.

I will then show how these OT mesh generation methods are implemented on both the plane and on the sphere by solving the Monge-Ampére or Monge-Ampére like equations by using fast quasi Newton methods.

In particular I will look at the solution of Poisson's equation in a non convex domain with re-entrant corners. Such problems are known to have singular solutions leading to large solution errors. I will show how optimal transport methods can be used to quickly generate meshes for solving these problems. Such meshes have scale independent regularity and lead to optimal error estimates despite the singularities in the solution of the PDE.

On thermodynamically compatible schemes for turbulent shallow water flows
Saray Busto (University of Trento), M. Dumbser, K. Ivanova, S. Gavrilyuk
Mon 14:50-15:15 R1.23 Z3

In this talk we will present a new reformulation of the first order hyperbolic model for unsteady turbulent shallow water flows recently proposed by *Gavrilyuk et al. 2018*. As a novelty, a novel formulation is proposed introducing a new evolution variable that guarantees the trace of the discrete Reynolds stress tensor to be always non-negative, *Busto et al. 2021*. The mathematical model is particularly challenging because one important subset of evolution equations is nonconservative and the nonconservative products also act across genuinely nonlinear fields. Therefore, we will first consider a thermodynamically compatible viscous extension of the model that is necessary to define a proper vanishing viscosity limit of the inviscid model and that is absolutely fundamental for the subsequent construction of a thermodynamically compatible numerical scheme. Then we will introduce two different, but related, families of numerical methods for its solution. The first scheme is a provably thermodynamically compatible semi-discrete finite volume scheme that makes direct use of the Godunov form of the equations resulting on the so-called discrete Godunov formalism. The new method mimics the underlying continuous viscous system exactly at the semi-discrete level and is thus consistent with the conservation of total energy, with the entropy inequality and with the vanishing viscosity limit of the model. The second scheme is a general purpose high order path-conservative ADER discontinuous Galerkin finite element method with *a posteriori* subcell finite volume limiter that can be applied to the inviscid as well as to the viscous form of the model. Both schemes have in common that they make use of path integrals to define the jump terms at the element interfaces. The different numerical methods are applied to the inviscid system and are compared with each other and with the scheme proposed in *Gavrilyuk et al. 2018* for different Riemann problems. Moreover, we make the comparison with a fully resolved solution of the underlying viscous system in the vanishing viscosity limit. In all cases an excellent agreement between the different schemes is achieved. We will furthermore show numerical convergence rates of ADER-DG schemes up to sixth order in space and time and present challenging test problems for the model where we also compare with available experimental data.

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Isomeric trees with applications to Runge-Kutta methods

John Butcher (University of Auckland)

Wed 08:00-08:10 R3.07, R3.28 @ Z1

Classical Runge–Kutta methods, up to the work of Nyström, were derived to achieve a required order for scalar problems, even though they often retained the same asymptotic accuracy for high-dimensional problems. By writing trees in terms of products of what will be referred to as atomic factors, the distinction between scalar and vector conditions is seen to be equivalent to identifying permuted products with the same factors. These interrelated trees are said to be "isomeric".

The number of conditions for order p, in the scalar and vector cases, are shown in the table below. Also shown are the number of free parameters for an s stage method, where s corresponds to the minimum number of stages to achieve order p.

p	scalar	vector	s	parameters
1	1	1	1	1
2	2	2	2	3
3	4	4	3	6
4	8	8	4	10
5	16	17	6	21
6	31	37	7	28

For $p = 5$, methods exist which have this order for a scalar problem, but not for a vector problem.

The first method of order 6, derived by A. Huťa, used $s = 8$ stages, so that there would be 36 parameters, which were expected, at that time, to be necessary to satisfy the 31 conditions for a scalar problem.

Uniformly accurate low regularity approximations for the Klein-Gordon equation and Klein-Gordon-Schrödinger systems

Maria Cabrera Calvo (Sorbonne University), Katharina Schratz

Tue 11:40-12:05 R3.28 Z2

We propose a novel class of uniformly accurate integrators for the Klein–Gordon equation and Klein-Gordon-Schrödinger systems which capture classical $c = 1$ as well as highly-oscillatory non-relativistic regimes $c \gg 1$ and, at the same time, allow for low regularity approximations. In particular, our first- and second-order schemes require no step size restrictions and, in addition, lower regularity assumptions than classical schemes, such as splitting or exponential integrator methods. Furthermore, the new schemes preserve the nonlinear Schrödinger (NLS) limit on the discrete level.

This is joint work with Katharina Schratz (Sorbonne University).

A class of spectral methods for deterministic and stochastic fractional differential equations.

Angelamaria Cardone (University of Salerno), Kevin Burrage, Raffaele D'Ambrosio, Beatrice Paternoster

Tue 17:10-17:50 R3.28 Z2

In time fractional models, the solution depends on all its past history; therefore such models are able to describe many evolutionary problems with memory. On the other hand, the numerical simulation by step-by-step methods (typically finite difference schemes) is computationally expensive. As a matter of fact, step-by-step methods represent a local approach, while fractional derivatives can be seen as global operators. In this perspective, we propose a spectral approach, which is a global scheme and avoids the discretization of the heavy tail of the solution at each time step. Moreover, spectral methods may exhibit an exponential error decay for a suitable choice of the spectral basis functions, while step-by-step methods usually have low order of convergence. In this talk, we illustrate a class of spectral methods for time fractional diffusion systems and for stochastic differential equations. We construct these methods and illustrate the linear steps which constitute their computational kernel. Then, we show their effectiveness on some test problems. Finally, we draw some conclusions and suggest possible developments.

Some Properties of Higher Order Differential Algebraic Equations with Singular Points

Elena Chistyakova (Institute for System Dynamics and Control Theory of Siberian Branch of Russian Academy of Sciences), V.F. Chistyakov

Tue 11:10-11:20 R1.23 Z3

In this talk, we consider systems of ordinary differential equations of arbitrary order with an identically singular matrix multiplying the higher derivative of the desired vector-function. Special attention is paid to the systems with singular points in the domain. We provide a formal definition of singular points and their classification. The criteria for the presence (absence) of singular points on the interval of integration has been formulated. A number of examples are given to illustrate theoretical results.

This research has been supported by the Russian Foundation for Basic Research, Project Nos. 20-51-54003, 18-29-10019.

Numerical Solution of two-dimensional parabolic SPDEs using a Galerkin exponential time differencing scheme combined with a boundary integral formulation

Julian Clausnitzer (Forschungszentrum Jülich GmbH), Andreas Kleefeld

Thu 14:30-15:00 R3.28 Z2

In this talk, we consider the numerical solution of two-dimensional parabolic stochastic partial differential equations (SPDEs). While the research on theory as well as numerics of SPDEs is growing rapidly, little to no effort has been made to solve SPDEs on two-dimensional domains that are more general than a rectangle. In this work, we aim to solve SPDEs on the much more general class of star-shaped domains by using a numerical Galerkin scheme developed by Jentzen and Kloeden in 2008. The scheme approximates the solution as a truncated Fourier sum with coefficients that vary in time, with a suitable orthonormal basis of the space of square integrable functions on the domain under Dirichlet boundary conditions. We use the Dirichlet eigenfunctions as a basis, which we find via translating the problem into a boundary integral formulation involving a double layer potential. The density in this layer potential as well as the

boundary of the domain are approximated piecewise using quadratic Lagrange polynomials. The resulting discretized nonlinear eigenvalue problem can be reduced to a linear eigenvalue problem and then solved using Beyn's integral algorithm. We will present examples for the numerical solution of an SPDE on two-dimensional domains, as well as an outline of an error analysis and possible applications.

Time integration of the stochastic Manakov equation
David Cohen (Chalmers University of Technology and University of Gothenburg)
Thu 17:30-18:00 R3.28 Z2

We present and analyze two efficient time integrators for the stochastic Manakov equation, a system arising in the study of pulse propagation in randomly birefringent optical fibers.
The presentation is based on joint works with André Berg and Guillaume Dujardin.

Geometric integration for the formation control of multi-agent systems
Leonardo Colombo (Instituto de Ciencias Matematicas (CSIC-UAM-UCM-UC3M)), David Martin de Diego
Tue 10:50-11:00 R1.23 Z3

Formation control of autonomous agents can be seen as a physical system of individuals interacting with local potentials, and whose evolution can be described by a Lagrangian function. We construct variational integrators for the formation control of autonomous agents modeled by double integrators. In particular, we find error estimations for the rate of the energy dissipated along with the agents' motion to achieve desired formations. Consequently, this permits to provide sufficient conditions on the time step for the convergence of discrete formation control systems such as the consensus problem in discrete systems.
We present practical applications such as the rapid estimation of regions of attraction to desired shapes in distance-based formation control. In addition, a Noether theorem for this class of systems is obtained, giving rise to an intrinsic geometric understanding of the exponential decay for the constants of the motion of the agents, in particular, linear and angular momentum.

Recent advances in deterministic and stochastic numerics for evolutive problems
Dajana Conte (Department of Mathematics, University of Salerno)
Fri 08:10-09:00 R3.07, R3.28 @ Z1

This contribution regards the numerical solution of evolutionary problems related to natural phenomena and physical processes modelled by functional equations of various type, with specific characteristics such as: stiffness, oscillations, presence of memory together with stochastic terms, by focusing especially on stability properties of the methods. We will describe the construction of adapted numerical methods, that is, strongly oriented to the problem and with excellent stability properties, where the stability will be also interpreted as preservation of the intrinsic qualitative characteristics of the problem itself.
For the numerical solution of stiff problems, originating for example from convection and diffusion terms in Partial Differential Equations (PDEs), methods with good stability properties can be obtained by exploiting the usage of the Jacobian matrix of the problem [1, 5]. Recent works on Time-Accurate and Highly-Stable (TASE) operators [2] show as the employment of these operators, together with explicit Runge-Kutta methods, can lead to A-stable schemes with a considerable gain in efficiency. We will focus our attention on the class of explicit and parallel peer methods [8, 9] combined with TASE operators, describing the derivation of highly

stable numerical methods.
For problems with oscillating solution, we will show how the use of non-polynomial bases reveals a powerful tool for adapting numerical methods to the known behavior of the solution [3, 4, 7].
For problems with memory and influenced by stochastic phenomena, modeled by stochastic Volterra integral equations, the focus will be on the construction of numerical methods that can inherit good stability properties from the methods for stochastic differential equations [6].
The presented results have been obtained in collaboration with Beatrice Paternoster, Leila Moradi and Giovanni Pagano (University of Salerno), Raffaele D'Ambrosio (University of L'Aquila), Liviu Ixaru (Institute of Physics and Nuclear Engineering, Bucharest), Fakhrodin Mohamadi (University of Hormozgan, Iran), Ali Abdi (University of Tabriz, Iran).

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Efficient nonlinear modeling of highly flexible beam structures using geometrically exact beam models

Marielle Debeurre (Arts et Metiers Institute of Technology), Aurélien Grolet, Olivier Thomas, Pierre-Olivier Mattei, Bruno Cochelin

Tue 17:30-18:00 R1.23 Z3

The study of highly flexible beam structures continues to be a subject of research as their behavior in bending often leads to complex nonlinear phenomena that can be difficult to model. Examples of such structures include cables, wires and ropes, where a simple, one-dimensional structure and low stiffness in bending combine to result in extreme deformation when subjected to certain loadings. A geometrically exact beam model is ideal for capturing the nonlinear behavior of flexible structures, yet more research is needed to improve the computational efficiency of existing solution strategies. We propose a novel method for the periodic solution of geometrically exact beam structures using a custom continuation algorithm instead of the usual solving schemes.

The defining feature of the geometrically exact beam model, as the name suggests, is the fact that all geometrical nonlinearities ($\sin\theta$ and $\cos\theta$) governing the rotation of the beam are kept exact without simplification [1]. The geometrically exact model is therefore capable of accurate representation even if the beam undergoes extreme displacement, as is the case with many flexible structures. A disadvantage of this model, however, is its complexity. Widely-used techniques for nonlinear dynamic simulation require a significant computational load when using the geometrically exact model, a load which will increase with the desired accuracy of the simulation. Instead, a newer technique for the dynamic simulation of nonlinear structures will be presented with several test cases shown.

The strategy first involves a finite element discretization of the beam systems based on the weak form variational formulation of the geometrically exact beam equations. In the case of the current plane stress condition, the system is reduced to 2D geometrically exact beam elements [2]. The weak form of the equations of motion are developed using simplified Green-Lagrange strains and linear Kirchhoff-Saint-Venant constitutive laws. The details of the finite element model can be found in [3]. The finite element model is then implemented into the interactive path-following solver, MANLAB. MANLAB combines the harmonic balance method (HBM) with the asymptotic numerical method (ANM) continuation technique for efficient solution of periodic systems [4, 5]. Advances in this technique and its application to various beam structures will also be presented.

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Long-term analysis of stochastic Hamiltonian systems under time discretizations

Stefano Di Giovacchino (University of L'Aquila), Raffaele D'Ambrosio University of L'Aquila

Thu 17:00-17:30 R1.23 Z3

In this talk, we focus our investigation on providing long-term estimates of the Hamiltonian deviation computed along numerical approximations to the solutions of stochastic Hamiltonian systems, both of Itô and Statonovich types. It is well-known that the expected Hamiltonian of an Itô Hamiltonian system with additive noise exhibits a linear drift in time [2], while the Hamiltonian function is conserved along the exact flow of a Stratonovich Hamiltonian system [3, 4]. Here, we address our attention to providing modified differential equations associated to suitable discretizations for above problems, by means of weak backward error analysis arguments [1, 5, 6]. Then, long-term estimates are provided both for Itô and Stratonovich Hamiltonian systems, revealing the presence of parasitic terms affecting the overall conservation accuracy. Finally, selected numerical experiments are provided to confirm the theoretical analysis. This talk is based on a joint work with Raffaele D'Ambrosio (University of L'Aquila).

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On structure-preserving schemes for continuum mechanics

Michael Dumbser (University of Trento), Saray Busto, Ilya Peshkov, Evgeniy Romenski, Walter Boscheri

Mon 09:00-09:50 R3.07, R3.28 @ Z1

We present two new structure-preserving schemes for symmetric hyperbolic and thermodynamically compatible (SHTC) systems with involution constraints. First, we present a new staggered semi-implicit method that is able to preserve curl constraints exactly on the discrete level and which is also compatible with the stiff relaxation limit of the governing equations. In the second part of the talk we present a new thermodynamically compatible finite volume scheme that is exactly compatible with the overdetermined structure of the model at the semi-discrete level, making use of a discrete form of the continuous formalism introduced by Godunov in 1961 (semi-discrete Godunov formalism).

MISSILES: an Efficient Resolution of the Co-simulation Coupling Constraint on Nearly Linear Differential Systems through a Global Linear Formulation

Yohan Eguillon (Institut Camille Jordan UMR5208-U.Lyon1-CNRS), Bruno Lacabanne, Damien Tromeur-Dervout

Mon 17:30-17:55 R3.07 Z1

In a co-simulation context, interconnected systems of differential equations are solved separately but they regularly communicate data to one another during these resolutions. Iterative co-simulation methods have been developped in order to enhance both stability and accuracy. Such methods imply that the systems must integrate one or more times per co-simulation step (the interval between two consecutive communications) in order to find the best satisfying interface values for exchanged data (according to a given coupling constraint).
MISSILES is a non-iterative method that leads to the same solution than an iterative co-simulation method (IFOSMONDI-JFM [1]), given a few hypothesis.
Through a transformation of the problem, an equivalent linear formulation of the global coupling constraints can be achieved. Hence, a single resolution leads directly to smooth (C1) and non-delayed interface signals satisfying the global coupling constraint of the co-simulation problem. This method can be used with systems that are not rollback-capable. In other words, systems that cannot integrate more than once a co-simulation step are not a limitation for the MISSILES algorithm. The main underlying hypothesis for this method is that the outputs of the differential systems can be written as a linear expression of the internal states variables and the coefficients of the polynomial of every input. Such a formulation can be achieved with a method based on the transfer function (in the Laplace domain): the COSTARICA[1] process. The later is very reliable on linear systems, and can be corrected regularly according to regular successive linearizations for non-linear systems. As a consequence, applications to multibody mechanical systems are feasible and promising. Regarding non-linear systems, a similar process can at least be used as a convenient predictor for non-iterative co-simulation algorithms as it does not imply integrations of the systems.

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Sub-linear convergence of a tamed stochastic optimization method

Monika Eisenmann (Lund University), Tony Stillfjord

Wed 11:10-11:20 R3.28 Z2

In order to solve a minimization problem, a possible approach is to find the steady state of the corresponding gradient flow initial value problem through a long time integration. The well-known stochastic gradient descent (SGD) method then corresponds to the forward Euler scheme with a stochastic approximation of the gradient. Our goal is to find more suitable schemes that work well in the stochastic setting.
In the talk, we present a stochastic version of the tamed Euler scheme in this context. This method is fully explicit but is more stable for larger step sizes compared to the standard SGD method. We provide convergence results with a sub-linear rate also in an infinite-dimensional setting. We will illustrate the theoretical results on numerical examples. A typical application for such optimization problems is supervised learning.

[1] Cautiously Obtrusive Solution To Avoid Rollback in Iterative Co-simulation Algorithms

Numerical methods for conservation laws on graphs

Ulrik Skre Fjordholm (University of Oslo), Markus Musch, Nils Henrik Risebro

Thu 09:00-09:50 R3.07, R3.28 @ Z1

We consider a set of scalar conservation laws on a graph. Based on a choice of stationary states of the problem – analogous to the constants in Kruzkhov's entropy condition – we establish the uniqueness and stability of entropy solutions. For rather general flux functions we establish the convergence of an easy-to-implement Engquist–Osher-type finite volume method.

High-order adaptive loose coupling of semi-discretised PDEs connected through interfacial conditions

Laurent Francois (ONERA), Joël Dupays, Marc Massot

Mon 17:55-18:20 R3.07 Z1

Detailed multiphysical simulations are required to accurately describe the combustion chamber dynamics inside a solid rocket motor (SRM). This class of motor relies on the combustion of a solid material, the solid propellant, which emits gaseous products as its surface melts. These products react and form a flame that sustains the combustion. The simulation of the ignition of a SRM requires a time accurate-coupling between two solvers: a CFD solver for the internal flowfield inside the combustion chamber, and thermal solver which determines the temperature profile inside the solid material [2]. These solvers exchange fluxes (mass, energy) as well as other variables (pressure). Early versions of this coupling have been reported, e.g. [1], however it is only first-order in time, which may cause precision loss while also hindering computational efficiency.

The problematic is close to the one of *conjugate heat transfer* (CHT) where an inert material is heated by a gas flow over its surface, however the solid propellant material introduces additional difficulties, such as the presence of algebraic equations for the propellant surface equilibrium, as well as stiff source terms related to the combustion. In the CHT framework, simulations are usually conducted by coupling the solvers at regular intervals. Considering the large computational cost associated with each solver, along with other technical limitations (inability to restart a time step, code complexity), most reported couplings are explicit and never reject a coupling step. Moreover, ensuring the conservativity of the physical exchanges at the surface of the solid material is not trivial [4]. Work has been reported on time adaptive coupling [3] where an error estimate is formed similarly to that of a multistep method, allowing for the time step to be dynamically adjusted.The overall coupling however remains first-order in time. It may be advantageous in terms of precision and computational efficiency to develop a coupling method that can be of higher-order.

In the present contribution, we introduce a new approach that allows a high-order explicit coupling of multiple subsystems that are connected via interfacial conditions, while natively providing an error-estimate for the selection of the coupling time step. This approach, based on polynomial extrapolation of the coupling variables and fluxes, is similar to specific methods that have been applied in the fields of computational mechanics. Each coupling variable is extrapolated in time based on a polynomial fit of several previous coupling steps. Each subsystem is integrated forward in time separately during one coupling time step, using these polynomial extrapolations as predictions of the coupling variables. The order (i.e. stencil length) of the polynomial fit is varied dynamically to improve stability and efficiency. The coupling time step is dynamically adapted so that an error estimate remains within prescribed bounds.

From a technical point of view, the implementation is straightforward and does not require intrusive code adaptation. We focus on simple test cases to present the method. The conservativity (energy, mass...) of the coupling is also discussed. A simplified model of the ignition of a solid rocket motor is used to demonstrate the efficiency of the approach.

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Exponentially Fitted Methods that Preserve Conservation Laws

Gianluca Frasca-Caccia (Università degli Studi di Salerno), Dajana Conte

Wed 10:50-11:00 R3.07 Z1

The solutions of PDEs modelling physical phenomena, typically satisfy a set of conservation laws. Conservation laws usually refer to some quantity with a precise physical meaning such as mass, momentum, energy or charge. They state that the change in the quantity within an arbitrary small region of the spatial domain, is given by the net amount of quantity that flows in or out of the volume.
From a mathematical point of view, conservation laws are among the most important geometric properties of a PDE and preserving them in the discrete setting confers local constraints on the behaviour of the numerical solutions and yields better accuracy over long integration times [3, 4].
When the solution has an oscillatory behaviour, it is well-known that exponentially fitted numerical methods perform much better than standard ones [1, 2]. In this talk we shall discuss a new technique to find exponentially fitted methods that preserve conservation laws. Numerical tests showing the effectiveness and conservative properties of the new methods will be presented.

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Convergence of the Neumann-Neumann Method for the Cahn-Hilliard Equation
Gobinda Garai (Ph.D student)
Wed 11:20-11:30 R3.07 Z1

In this paper, we analyze a substructuring type algorithm for the Cahn-Hilliard (CH) equation. Being a nonlinear equation, it is of great importance to develop efficient numerical schemes for investigating the solution behaviour of the CH equation. We present the formulation of Neumann-Neumann (NN) method applied to the CH equation and investigate the convergence behaviour of the same in one and two spatial dimension for two subdomains. We illustrate the theoretical results by providing numerical example.

A change of perspective in variable-order fractional calculus
Roberto Garrappa (University of Bari), Andrea Giusti, Francesco Mainardi
Tue 14:50-15:30 R3.28 Z2

In the last two or three decades different approaches to introduce fractional integrals and derivatives of variable-order have been investigated. Fractional variable-order operators are indeed useful to model a series of physical phenomena in which persistent memory effects or anomalous properties change over time and/or space.
Starting from some preliminary ideas by the Italian engineer Giambattista Scarpi, in this talk we present a new approach for generalizing standard fractional operators of constant order α to variable order $\alpha(t)$. Rather than operating directly in the time domain, the proposed approach performs the generalization in the Laplace transform domain. Moreover, the obtained variable-order differential and integral operators are framed in the robust mathematical theory of General Fractional Derivatives and Integrals relying on the Sonine condition.
The absence of an analytical time-domain representation of these variable-order operators forces us to an extensive use of numerical methods for the inversion of the Laplace transform and for the solution of differential equations which will be discussed in details.

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Training neural networks with corrected Langevin dynamics and stochastic gradients
Adrià Garriga-Alonso (University of Cambridge)
Tue 17:00-17:30 R3.07 Z1

The last decade has popularised a family of Markov chain Monte Carlo (MCMC) algorithms for training Bayesian neural networks. These algorithms are numerical solutions to the Langevin stochastic differential equations of various orders, where the potential function is related to the neural network and training data. In order to computationally scale to the large training data sets common in modern machine learning (ML), the algorithms use stochastic estimates of the potential's gradient.
To ensure that MCMC converges to the target probability distribution, one needs to correct for discretisation errors using a ratio of density functions. Calculating this ratio requires a pass over the whole data set. Common wisdom in Bayesian ML holds that it is prohibitive to perform this correction at every step, so the sampler is used without correction instead. As a result, we are left with no correctness guarantees, and no way to monitor the error of our samples from the target.

In this talk I show that it is possible to exactly perform the correction step while using stochastic gradients. The exact ratio evaluation is performed only after many gradient steps, thus introducing only a small (2-5%) slowdown compared to the uncorrected algorithm, or to mainstream neural network training algorithms like stochastic gradient descent. This allows the practitioner to monitor the approximation error, or to eliminate it completely at extra computational cost. The correction is applicable to most semi-implicit discretisation schemes.

Continuous-time extensions of stochastic one-step methods

Giuseppe Giordano (University of Salerno), Dajana Conte, Raffaele D'Ambrosio, Beatrice Paternoster

Wed 11:00-11:10 R3.28 Z2

In this work we focus our attention on the development of continuous extensions to stochastic one-step methods for the time discretization of Stochastic Differential Equations (SDEs) [1, 2]

$$X(t) = X(t_0) + \int_{t_0}^{t} f(X(s))ds + \int_{t_0}^{t} g(X(s))dW(s), \quad t \in [t_0, T], \tag{1}$$

where $W(t)$ is a multidimensional standard Wiener process. Inspired by the idea of deterministic numerical collocation [5, 6], we provide a continuous time extension of stochastic one-step methods, by imposing that the solution of (1) can be approximated with a piecewise linear polynomial. A dense numerics output allows to provide a more efficient error estimate and it is a very effective for a variable step-size implementation [4]. We show the constructive technique and provide selected numerical experiments confirming the effectiveness of the proposed approach.

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High order PDE-convergence of AMF-W methods for parabolic problems

Severiano Gonzalez Pinto (Universidad de La Laguna), E. Hairer, D. Hernández-Abreu

Mon 17:30-17:55 R1.23 Z3

The PDE-orders of convergence in the Euclidean norm of s-stage AMF-W-methods for two dimensional parabolic problems on rectangular domains are considered. We explain the algebraic conditions to reach order three in the case of homogeneous Dirichlet boundary conditions and give some interesting methods having that order. We also provide some evidence that seems to indicate that PDE-convergence of order four cannot be achieved with that kind of method.

Lift and flow: manifold MCMC methods for efficient inference in stiff posteriors

Matt Graham (University College London), Au Khai Xiang, Alexandre Thiery

Tue 15:00-15:30 R3.07 Z1

A challenging regime for employing Markov chain Monte Carlo (MCMC) methods to perform Bayesian inference is when the observed data tightly constrains only some directions in the latent space. Such 'stiff' posterior distributions have varying scales across the latent space and can exhibit complex geometries. The posterior mass may concentrate near lower-dimensional structures in the latent space and funnel-like pathologies can emerge where the distribution can vary between highly concentrated and highly diffuse regimes due to poor identification of scale parameters. As the step size parameter of MCMC methods typically needs to be set according to the smallest posterior scale to ensure chains can access all parts of the distribution, this can lead to slow exploration of less constrained directions or regions of the posterior. In this talk I will discuss an approach for constructing efficient Markov kernels targeting such posteriors when the underlying generative model is differentiable. The posterior distribution is lifted on to a manifold embedded in a higher dimensional space, and then a Hamiltonian flow, constrained to the manifold, simulated to generate proposed moves. In contrast to the original posterior the lifted distribution remains diffuse in the presence of highly informative observations, allowing the constrained Hamiltonian flow to be simulated with a large integrator step size and for chains to rapidly mix in the lifted distribution. As we demonstrate empirically, this can lead to substantial improvements in sampling efficiency over competing approaches.

Error analysis for Galerkin-BDF discretizations of nonlinear differential-algebraic systems of index-1 with an elliptic operator constraint

Dennis Groh (Humboldt-Universität zu Berlin), Caren Tischendorf

Mon 16:40-17:05 R3.28 Z2

The dynamics of flow networks (e.g. circuits) can often be described by a differential-algebraic system (DAE). However, it is restricted to lumped network element models. If spatial effects can not be neglected, distributed element models have to be included. Here, we are interested in networks that include distributed elements of elliptic type. Therefore, we consider index-1 DAEs of the form

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} m(x(t),t) + f(x(t),y(t),u(t),t) &= 0, \\ g(x(t),y(t),t) &= 0 \end{aligned}$$

coupled with a constraint of the form

$$\mathcal{B}(u(t)) + \mathcal{R}(x(t),y(t),t) = 0$$

where $\mathcal{B}\colon V \to V^*$ is a strongly monotone and hemicontinuous operator and V is a separable Banach space. Under some additional monotonicity and Lipschitz assumptions, we present an error analysis for discretizations of such systems based on a Galerkin approach for the operator constraint and the BDF method for the time discretization of the full system.

Modelling and Simulation of the Convection-Diffusion Equation through Fractional Restricted Calculus of Variations

Emina Hadzialic (University of Paderborn), Sina Ober-Blöbaum, Fernando Jimenez Alburquerque, Jacky Cresson

Thu 13:30-14:00 R1.23 Z3

Using variational formulations is a common way to characterise equations. Moreover, it is also convenient to apply variational methods in order to develop numerical schemes. In this work we are focusing on dissipative systems. Classical variational tools do not apply to these, which leads to difficulties in the numerical study of the corresponding equations. Thus, we are proposing to look for a generalised variational setting, a new kind of fractional calculus of variations, called "restricted calculus of variations", allowing to deal with these equations. More precisely, we define a phase space including the fractional derivative of curves and, furthermore, we use a particular restriction upon the admissible variations. Moreover, a variational discretisation yields particular numerical schemes, called variational integrators, which, thanks to their powerful structure-preserving properties, have already shown superior performance in different scenarios, like conservative systems. In this talk we are going to introduce our preliminar continuous results about how to obtain the well-known convection-diffusion equations employing this approach. In this way, we are able to provide a fractional Lagrangian formulation of the convection-diffusion equation. We shall show that the fractional variational formulation leads to a family of fractional convection-diffusion equations. In other words, the method provides a more general expression. We will finish the presentation by showing some numerical results of our implementation.

Numerical Affine Lower Bound for Polynomials over Simplices with Applications

Tareq Hamadneh (Al Zaytoonah University of Jordan), Mohammad Obeida

Mon 15:15-15:40 R1.23 Z3

We investigate the problem of finding tight affine lower bounding functions for multivariate polynomials over a given simplex. These functions are obtained by using the expansion of the given polynomials into Bernstein form. Convergence forms to polynomials are given with respect to raising the degree and number of subdivision steps. We present a method for constructing linear affine lower bounding functions for multivariate polynomial functions based on the control points, the convex hull of Bernstein control points and degree elevation. Convergence forms and Monotonicity of the minimum error bounds are investigated. finally, application to global optimization and stability of control polynomial functions is addressed.

Discretization of a phase field model

Maren Hantke (Martin Luther University Halle-Wittenberg), Hazem Yaghi, Gerald Warnecke

Fri 10:50-11:40 R3.07, R3.28 @ Z1

In our presentation we will discuss a phase field model introduced in 2014. This model was proposed to describe chemically reacting fluid mixtures consisting of N constituents where phase transitions between a liquid and a vapor phase may occur. The phase field indicates the present phase or the transition layer. The discretization of the model is a challenge for several reasons. Difficulties arise for instance from steep gradients in the density as well as from the nature of the phase field quantity. We will focus on this in our presentation.

Spatial nonlinear beam theory for soft pneumatic actuators

Jonas Harsch (Institute for Nonlinear Mechanics - University of Stuttgart), Giuseppe Capobianco, Simon R. Eugster

Tue 15:00-15:30 R1.23 Z3

In the emerging research field of soft robotics recent investigations examine how cylindrical beam like structures made of silicone can be described using spatial nonlinear beam theories. These structures are frequently actuated by inflating multiple eccentrically embedded pressure chambers. The talk extends the classical spatial nonlinear beam theories, given in the variational framework of the principle of virtual work, by pressurized chambers. This contains the formulation of the internal virtual work contribution of the pressurized medium which is restricted to the beam-like kinematics of the enveloping material. Using the principle of virtual work, which demands the total virtual work to vanish for all admissible virtual displacements, the equilibrium equations follow by an integration by parts procedure. The silicone's elastic material response is modeled by using a nonlinear Ogden-like material law for the beam's axial direction. Further, the radii of the embedded pressure chambers are linearly coupled with the applied pressure. The unknown material parameters of the proposed material laws are identified using an optimization procedure with respect to selected experimental measurements. The talk is completed by showing that the proposed model together with the identified material parameters is capable of reproducing the results of a different unknown experiment.

Systems with Stochastic Pattern Formation

Erika Hausenblas (Universitaet Leoben), Mechtild Thalhammer, Debopriya Mukherjee, Akash Panda,

Thu 17:00-17:30 R3.28 Z2

Mathematical models based on systems of reaction-diffusion equations provide fundamental tools for the description and investigation of various processes in biology, biochemistry, and chemistry; in specific situations, an appealing characteristic of the arising nonlinear partial differential equations is the formation of patterns, reminiscent of those found in nature. The deterministic Gray-Scott equations, or e.g. or Gierer Meinhardt model constitute an elementary two-component system that describes autocatalytic reaction processes; depending on the choice of the specific parameters, complex patterns of spirals, waves, stripes, or spots appear.
In the derivation of a macroscopic model from basic physical principles, certain aspects of microscopic dynamics, e.g. fluctuations of molecules, are disregarded; an expedient mathematical approach that accounts for significant microscopic effects relies on the incorporation of stochastic processes and the consideration of stochastic partial differential equations.
The randomness leads to a variate of new phenomena and may have a highly non-trivial impact on the behaviour of the solution. E.g. it has been shown by numerical modelling that the stochastic extension leads to a broader range of parameters with Turing patterns by a genetically engineered synthetic bacterial population in which the signalling molecules form a stochastic activator-inhibitor system. The stochastic extension may lead to multistability and noise-induced transitions between different states.
In the talk, we will introduce the Gray Scott system and Klausmeier system, which is a special case of an activator-inhibitor system. Then, we give shortly the proof of existence and uniqueness, and introduce its numerical modelling.

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On the construction of numerical integrators for ODEs based on the linear barycentric rational interpolants

Gholam Reza Hojjati (University of Tabriz), Ali Abdi

Mon 16:40-17:05 R3.07 Z1

The designing of traditional numerical integrators for ODEs are usually based on customary polynomial interpolants. Using of linear barycentric rational interpolants is an efficiency technique which leads to the construction of numerical methods with better accuracy and stability properties. In this talk, we introduce some family of classes of the first and second derivative multistep methods. The convergence, accuracy and stability properties of the constructed methods are discussed and verified by the numerical experiments.

A novel POD-DEIM-like model reduction method for the compressible Euler and Navier-Stokes equations

Zoltán Horváth (Széchenyi István University), Mátyás Constans

Tue 11:30-11:40 R1.23 Z3

We realized permanent failures of our computer code of the classical POD-DEIM by Chaturantabut-Sorensen and its QDEIM variant by Drmac-Gugercin when applied to 1st and 2nd order finite volume semi-discretizations of the 3D compressible Euler and Navier-Stokes equations with the ideal equation of states. Then we have introduced and applied a regression method instead of the interpolation step in DEIM, which resulted in a stable code.
In this talk, we present the new POD-DEIM-like reduced order method, overview its implementation, examine its accuracy, and provide results of some applications for external flow computations in complex domains in 3D.

Efficient methods for Volterra integro-differential equations based on Floater-Hormann interpolants

Seyyed Ahmad Hosseini (Golestan University), Ali Abdi

Mon 14:25-14:50 R3.07 Z1

One of the conventional and beautiful ways for the numerical solution of Volterra integro-differential equations (VIDEs) can be obtained using a combination of finite differences and quadrature rules, which, because of their efficiency, accuracy, and simplicity for the implementation, play an important role in the numerical study of such equations. This talk is devoted to deriving a highly accurate and stable scheme which is composed of left one-sided barycentric rational finite differences for approximating the derivative term and the composite barycentric rational quadrature for approximating the integral term.

Geometrically exact beam theory - Implementation based on automatic differentiation with the AceGen/AceFEM system

Toni Jelusic (C3M)

Tue 14:30-15:00 R1.23 Z3

The three-dimensional finite strain rod theory proposed by Simo [1] is the cornerstone for nonlinear analysis of slender structu res. An implementation of this theory is developed by using a symbolic-numeric approach. Automatic differentiation is used to obtain the der ivations of governing equations which are subsequently used in a finite element environment to carry out simulations of slender structures. The advantage of automatic differentiation (AD) is that it avoids the problem of expression growth that is associated with symbolic differen tiation. This is accomplished by searching for common subexpressions *during* derivation of equations and generation of numerical cod e [2], which results in better optimization of the code.
AceGen is used to generate C code containing the information about the governing equations of a physical problem. The AceGen system is based on the theory that combines automatic differentiation, simultaneous optimization of expressions with automatic selection and introduction o f appropriate intermediate variables. It's primary use is the derivation of equations for nonlinear finite element analysis. The derived gov erning equations are then used in finite element environments such as AceFEM, Abaqus or Ansys [3].
The advantage of the symbolic-numeric approach is the inclusion of governing equations in their full mathematical form, without any modifica tions used in numerical implementation. The numerical test cases of this implementation include the "Cantilever 45-degree 3D bend" [4], restrained to fixed end loads, and the case "Pure bending of a cantilever beam" [1].

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Stability analysis of multi-order fractional differential equations

Eva Kaslik (West University of Timisoara, Romania), Oana Brandibur, Roberto Garrappa

Tue 17:50-18:30 R3.28 Z2

In this talk, we review several results regarding the stability analysis of linear systems of fractional differential equations. Starting from the well-known results of Matignon on the stability of single-order systems, the presentation is geared towards multi-order systems, as well as linear multi-term fractional differential equations with Caputo derivatives. Discrete-time counterparts of the obtained results are also presented, in the framework of systems of fractional-order difference equations with Caputo-type differences.

Approximation of Functions and Solutions to Ordinary Differential Equations by Adaptive Poly-Sinc Methods

Omar Khalil (German University in Cairo), Maha Youssef (U Stuttgart, DE), Gerd Baumann (GUC, EG and U Ulm, DE)

Wed 11:10-11:20 R1.23 Z3

We propose an adaptive method based on Poly-Sinc approximation to approximate functions and to solve ordinary differential equations (ODEs). Poly-Sinc approximation is a Lagrange interpolation scheme in which non-equidistant points generated by conformal mappings are used. These non-equidistant points are called Sinc points, which are characterized by their dense distribution near the endpoints of a finite interval. We discuss the error analysis of the adaptive Poly-Sinc approximation and show that the algorithm has a convergence rate of exponential order. We test the adaptive Poly-Sinc approximation on continuous functions and functions with singularities at the endpoints of a finite interval.

We also propose an adaptive Poly-Sinc-based collocation method to approximate solutions to ODEs. We test the adaptive collocation method on ODEs whose exact solution exhibits a singularity at one endpoint of a finite interval and singular ODEs whose exact solution is a continuous function on a finite interval.

Pointwise-in-time a posteriori error control for time-fractional parabolic equations

Natalia Kopteva (University of Limerick)

Tue 16:30-17:10 R3.28 Z2

For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0,1)$, we give pointwise-in-time a posteriori error bounds in the spatial L_2 and L_∞ norms. Hence, an adaptive mesh construction algorithm is applied for the L1 method, which yields optimal convergence rates $2-\alpha$ in the presence of solution singularities.
The talk is based on the recent article: N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, Appl. Math. Lett., 2021, https://doi.org/10.1016/j.aml.2021.107515.

Computational aspects of the velocity based elements in post-buckling analysis of beams and frames.

Sudhanva Kusuma Chandrashekhara (University of Ljubljana), Dejan Zupan

Tue 18:00-18:30 R1.23 Z3

In the nonlinear stability analysis of structures undergoing complex deformation, the precise prediction of the behaviour of the structure in the post-buckling regime poses a serious challenge during the finite element analysis. The problem is multifold in nature and requires numerous calculation such as, precise identification and classification of critical points, identification of correct loading path etc. Near the critical points of the equilibrium path, the load-deflection characteristics are dynamic in nature and requires short time intervals to simulate quasi-static load increment. In addition, time dependent load-relaxation techniques are necessary for the structures exhibiting snap-through and snap-back behaviour. In the present work, we use the velocity based finite element formulation of a geometrically exact beam model with the extension of the equilibrium equation with a modified arc length constraint. The crucial idea of the formulation is to employ velocities in the fixed frame description and angular velocities in the moving frame description as the primary unknowns. The model allows the use of standard

additive type interpolation functions to be fully consistent with the configuration space. We present some preliminary results of the post-buckling analysis with suitable numerical examples. The present work serves as a starting point in the post-critical analysis of structures such as beams and frames.

Connecting random fields on manifolds and stochastic partial differential equations in simulations

Annika Lang (Chalmers & University of Gothenburg), David Cohen, Erik Jansson, Mihály Kovács, Mike Pereira

Thu 13:00-13:30 R3.28 Z2

Random fields on manifolds can be used as building blocks for solutions to stochastic partial differential equations or they can be described by stochastic partial differential equations. In this talk I present recent developments in numerical approximations of random fields and solutions to stochastic partial differential equations on manifolds and connect the two. More specifically, we look at the stochastic wave equation on the sphere and approximations of Gaussian random fields on manifolds using suitable finite element methods. Throughout the talk, theory and convergence analysis are combined with numerical examples and simulations.

Super-Convergent IMEX-Peer Methods with Variable Time Steps

Jens Lang (Technische Universität Darmstadt, Department of Mathematics), Moritz Schneider, Rüdiger Weiner

Mon 14:00-14:25 R3.07 Z1

Dynamical systems with sub-processes evolving on many different time scales are ubiquitous in applications. Their efficient solution is greatly enhanced by automatic time step variation. In this talk, I will present the theory, construction and application of IMEX-Peer methods that are super-convergent for variable step sizes and A-stable in the implicit part [5]. IMEX-Peer schemes – like other IMEX-methods as well – combine the necessary stability of implicit and low computational costs of explicit methods to efficiently solve systems of ordinary differential equations with both stiff and non-stiff parts included in the source term [1,2,3,4]. To construct super-convergent IMEX-Peer methods which keep their higher order for variable step sizes and exhibit favourable linear stability properties, we derive necessary and sufficient conditions on the nodes and coefficient matrices and apply an extrapolation approach based on already computed stage values. New super-convergent IMEX-Peer methods of order $s+1$ for $s = 2, 3, 4$ stages are given as result of additional order conditions which maintain the super-convergence property independent of step size changes. Numerical experiments and a comparison to other super-convergent IMEX-Peer methods show the potential of the new methods when applied with local error control.

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Stochastic two-dimensional neural field equation: numerical approximation and applications to working memory

Pedro Lima (Instituto Superior Técnico, University of Lisbon), W. Erlhagen, G.Yu. Kulikov, M.V. Kulikova

Tue 10:50-11:15 R3.28 Z2

The main goal of the present work is to investigate the effect of noise in some neural fields, used to simulate working memory processes. The underlying mathematical model is a stochastic integro-differential equation. In order to approximate this equation we apply a numerical scheme which uses the Galerkin method for the space discretization. In this way we obtain a system of stochastic differential equations, which are then approximated in two different ways, using the Euler-Maruyama and the Itô-Taylor methods. We apply this numerical scheme to explain how a population of cortical neurons may encode in its firing pattern simultaneously the nature and time of sequential stimulus events. Numerical examples are presented and their results are discussed.

A multirate variational approach to simulation and optimal control for flexible spacecraft

Yana Lishkova (University of Oxford), Sina Ober-Blöbaum, Mark Cannon, Sigrid Leyendecker

Thu 14:00-14:30 R1.23 Z3

In this talk we will focus on the advantages of using multirate discrete mechanics for the solution of optimal control problems. Through the example case study of optimal control for flexible satellites we will demonstrate that this methodology can lead to high fidelity solutions at a reduced computational cost.

The methodology, named Multirate Discrete Mechanics and Optimal Control (DMOC), is originally introduced by Gail et al. [1] and tested by means of simple examples whereas its analysis and further development are still open research topics. In this methodology, the description of the mechanical system, as well as the necessary optimality conditions are derived though a multirate discrete version of the Lagrange-d'Alembert principle. The resulting structure-preserving time-stepping multirate equations serve as equality constraints for the optimisation problem and allow for a discrete optimal control problem formulation, which inherits the conservation properties of the continuous-time model. The lower number of time nodes on which some of the generalized coordinates are computed reduces the number of unknowns in the optimisation as well as the dimensionality of the constraints. This results in lower computational cost compared to the single rate method while achieving comparable accuracy in the solution. Further reduction in the computational time and memory usage can be achieved by the exploitation of the resulting sparse structure in the Jacobians of the constraint and cost functions.

As we will demonstrate, this approach also allows for a formulation of the optimal control problem which avoids computation of the momentum during the optimisation process further reducing the number of constraints by half and the unknowns by more than a third depending

on the problem. Overall, we will showcase that this approach allows for great customization of the scheme to the time scales of the problem and achieves high computational savings for negligible penalty in the accuracy. These advantages and capabilities of the numerical scheme will be demonstrated through its application for the problem of simultaneous attitude and vibration control of flexible spacecraft.

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Adaptive timestepping for S(P)DEs.

Gabriel Lord (Radboud University, Nijmegen), C. Kelly, S. Campbell

Mon 10:50-11:40 R3.07, R3.28 @ Z1

Traditional explicit numerical methods to simulate stochastic differential equations (SDEs) or stochastic partial differential equations (SPDEs) rely on globally Lipschitz coefficients to ensure convergence. Many applications of interest include non Lipschitz drift functions. Implicit methods (when they exist) can often be too computationally expensive for practical uses and standard explicit methods suffer from growth of moments of the solution (which can be thought of as a form of numerical instability).
Therefore the construction of explicit methods to simulate SDEs or SPDEs with non-Lipschitz drift has been an area of great interest. These methods are broadly in a number of classes where either the numerical approximations are projected or the growth is controlled in the scheme.
In this talk we give an overview, emphasizing the context of SPDEs, of this issue and discuss how using an adaptive time step can be used to control this growth. We will discuss some of the key difficulties in proving strong convergence with a random time mesh and how these might be overcome. We show that in numerical experiments the adaptive time stepping is an efficient alternative to the other methods.

Learning nonlinear operators via DeepONet

Lu Lu (University of Pennsylvania)

Tue 14:00-14:30 R3.07 Z1

It is widely known that neural networks (NNs) are universal approximators of continuous functions. However, a less known but powerful result is that a NN with a single hidden layer can accurately approximate any nonlinear continuous operator. This universal approximation theorem of operators is suggestive of the structure and potential of deep neural networks (DNNs) in learning continuous operators or complex systems from streams of scattered data. We design a new network with small generalization error, the deep operator network (DeepONet). We demonstrate that DeepONet can learn various explicit operators, such as integrals and fractional Laplacians, as well as implicit operators that represent deterministic and stochastic differential equations. Furthermore, we extend DeepONet to DeepM&Mnet, a new data assimilation framework for simulating multiphysics and multiscale problems at speeds much faster than standard numerical methods.

Overdetermined least-squares collocation for higher-index differential-algebraic equations

Roswitha März (Institut für Mathematik, Humboldt-Universität zu Berlin)

Mon 17:30-17:55 R3.28 Z2

This is again a joint effort with Michael Hanke (KTH Stockholm) and ties in with the results we both presented at NUMDIFF-15.
We are looking for an approximate solution $x_\pi \in X_\pi$ of the initial- or boundary-value problem

$$f((Dx)'(t), x(t), t) = 0,\ t \in [a, b], \quad g(x(a), x(b)) = 0.$$

The DAE in it can be of arbitrarily high index. The ansatz-space X_π consists of componentwise and piecewise polynomial functions x_π on the grid $\pi : a = t_0 < t_1 < \cdots < t_n = b$, with continuously connected part Dx_π. We use polynomials of degree $N > 1$ for the component Dx_π but for the nondifferentiated part degree $N - 1$. Introducing $M \geq N + 1$ so-called collocation nodes $0 \leq \tau_1 < \cdots < \tau_M \leq 1$ and in turn $t_{ji} = t_{j-1} + \tau_i h_j$, we form the overdetermined collocation system

$$f((Dx_\pi)'(t_{ji}), x_\pi(t_{ji}), t_{ji}) = 0,\ i = 1, \ldots M,\ j = 1, \ldots n, \quad g(x_\pi(a), x_\pi(b)) = 0,$$

which is then solved into a special least-squares sense for x_π. The procedure is inherently simple, the numerical tests are surprisingly good, but the underlying theory is quite demanding. Considering the fact that we are dealing here with an essentially ill-posed problem, it is important to implement it very carefully. Many questions are still open. We describe achievements, difficulties and surprises.

Convergence analysis of least-squares oversampled collocation for boundary element methods

Georg Maierhofer (Laboratoire Jacques-Louis Lions, Sorbonne University), Daan Huybrechs

Tue 11:15-11:40 R3.07 Z1

Collocation methods for boundary integral formulations of partial differential equations are simpler and cheaper to implement than Galerkin methods because the elements of the discretisation matrix are given by lower-dimensional integrals. However, in general, their application is a delicate matter: in contrast to Galerkin methods, there is no standardised convergence theory for collocation methods, and their success is sensitive to the choice of collocation points. Moreover, in the integral equation setting, collocation methods typically lead to slower convergence rates than Galerkin methods.
In this talk, we explore the extent to which the convergence properties of collocation methods for Fredholm integral equations can be improved by least-squares oversampling. We show that superlinear oversampling can enhance the convergence rates of the collocation method and reduce its sensitivity to the distribution of collocation points. In addition, we prove that linear oversampling can still lead to a substantial improvement in the error constant, even though the asymptotic convergence rate is not improved. Indeed, we will see an example where oversampling by a constant factor leads to an improvement of the error at a cubic rate in this constant, whilst incurring only a linear increase in cost. We support our analysis with several numerical examples for the two-dimensional Helmholtz equation.

Modeling of inelastic effects in composite cables by means of Hysteresis operators

Davide Manfredo (Fraunhofer ITWM), Vanessa Dörlich, Joachim Linn, Martin Arnold

Tue 17:00-17:30 R1.23 Z3

The present contribution aims at describing hysteresis behaviour arising from cyclic bending experiments on cables by means of the Preisach operator. As shown in pure bending experiments, slender structures such as electric cables behave inelastically and open hysteresis loops arise, with noticeable difference between the first load cycle and the following ones.
The Preisach operator plays an important role in describing the input-output relation in hysteresis behaviours and it can be expressed as a superposition of relay operators $\mathcal{R}_{s-r,s+r}[v](t)$

$$w(t) = \mathcal{P}[v](t) = \int_0^{+\infty} \int_{-\infty}^{+\infty} \omega(r,s)\mathcal{R}_{s-r,s+r}[v](t)dsdr.$$

The definition of the Preisach plane occurs naturally from the definition of Preisach operator and hysteresis loops can be computed by integrating a suitable kernel function $\omega(r,s)$ over a domain included in the Preisach plane, described by the variables r and s.
A mathematical formulation of the problem is introduced and a first attempt is made to mathematically determine the hysteresis behaviour that describes the relation between curvature (i.e. input $v(t)$) and bending moment (i.e output $w(t)$) of specific electric cables. Therefore, a suitable kernel function is identified in a way that its integration over the Preisach plane results in the bending moment of the specimen.

Geometric nonholonomic integrators

David Martin de Diego (Institute of Mathematical Sciences ICMAT), Alexandre Anahory Simoes, Sebastian Ferraro and Juan Carlso Marrero

Tue 11:00-11:10 R1.23 Z3

In this talk we will explore some new results in the construction of geometric integrators for a particuar type of constrained systems: nonholonomic mechanics where the dynamics is restricted by nonintegrable constraints on velocities. One of its most remarkable properties is that the derivation of the nonholonomic equations is not variational. However, we have recently discovered that mechanical nonholonomic systems may be seen as variational if we choose an appropriate Riemannian structure. In fact, we may show slightly more: its trajectories are geodesics relative to this structure so that, in particular, they are length minimizing! See Anahory Simoes, A., Marrero, J. C., Martín de Diego, D.: Radial kinetic nonholonomic trajectories are Riemannian geodesics!. arXiv:2010.12444, 2020.). We will define a Riemannian structure on this submanifold and show that nonholonomic trajectories starting at a fixed point q of the configuration space are geodesics relative to the new Riemannian manifold. The case of mechanical nonholonomic systems will not be addressed with detail because we also show that its trajectories are reparametrizations of that of kinetic nonholonomic system associated to the Jacobi metric.
Finally, we will discuss how this theoretical machinery may be used to construct geometric integrators for nonholonomic mechanics.

Recurrent Neural Networks inspired by ODEs
Siddhartha Mishra (ETH Zurich), T. Konstantin Rusch
Tue 13:30-14:00 R3.07 Z1

Recurrent neural networks (RNNs) are the neural network architecture of choice of learning tasks involving time series inputs and outputs such as natural language processing, speech recognition and time series analysis. It is very challenging to design RNNs that can learn tasks with long-term dependencies while still being expressive i.e., possess the ability of process complex inputs and outputs. We present a suite of RNNs that are inspired by dynamical systems, namely CoRNN (based on nonlinear coupled oscillators), UniCORNN (based on a Hamiltonian system) and LEM (based on a multi-scale ODEs) that are proved to mitigate the exploding and vanishing gradient problem and enable them to deal with tasks with very long-term dependencies. These architectures provide state of the art performance on a wide variety of learning tasks.

Augmented Lagrangian preconditioning for fluids: theory and practice
Lawrence Mitchell (Durham University)
Thu 13:00-13:30 R3.07 Z1

Augmented Lagrangian preconditioning for fluids problems was introduced by Benzi and Olshanskii in 2006. The approach offers excellent, parameter-robust, control of the Schur complement approximation. The drawback is that the preconditioning scheme for the top-left block is significantly more complicated, and at the time, an extension to three dimensions was not known. In recent years, there has been significant progress in this area, guided by a deeper understanding of how to construct appropriate preconditioners, and software advances that ease implementation.
The core idea in the design of effective preconditioners for the top left block is characterising a basis for the kernel of the augmented Lagrangian term. Structure preserving discretisations offer a systematic way to attack this problem when the augmentation is a differential operator. The resulting robust multigrid methods require small block overlapping additive Schwarz smoothers. In this talk I will discuss the general augmented Lagrangian approach, discuss a flexible preconditioning package that provides fast implementation of optimal methods, and illustrate with some examples covering stationary Navier–Stokes and MHD, along with time-dependent problems.

Long-time simulation of spherical hydrodynamics via quantization
Klas Modin (Chalmers and University of Gothenburg), Milo Viviani
Wed 08:10-09:00 R3.07, R3.28 @ Z1

Incompressible inviscid hydrodynamics on the sphere constitute a basic model in geophysical fluid dynamics. To understand the qualitative long-time behavior in such models is a fundamental problem in mathematical physics. The equations of motion possess a Poisson structure that gives rise to infinitely many conservation laws (Casimir functions) in addition to conservation of energy and momentum. To preserve this structure in discretizations is notoriously difficult, yet essential to capture the correct long-time behavior; the only known approach, due to Zeitlin (1991), is based on quantization theory. In this talk I show how Zeitlin's approach, developed for the flat 2-torus, can be adopted to the sphere. Indeed, for differential geometric reasons it works even *better* on the sphere than on the torus! Furthermore, the quantized equations themselves give new insights, such as a natural separation of variables that captures scale separation previously seen in both numerical simulations and direct observations of the atmosphere.

Frequency evaluation for adapted peer methods

Leila Moradi (University of Salerno), Dajana Conte, Beatrice Paternoster

Wed 11:00-11:10 R1.23 Z3

In this talk, we consider systems of Ordinary Differential Equations (ODEs) of the form

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0 \in \mathbb{R}^d, \quad t \in [t_0, T], \tag{1}$$

where $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently smooth to ensure that the solution exists and it is unique. We consider a general class of Exponentially Fitted (EF) two-step peer methods [5, 6] for numerical integration of ODEs (1) with oscillatory solution. EF algorithms for the numerical integration of problems with oscillating or periodic solutions are able to exploit the information about the frequency of oscillation in order to reduce the computational cost [1].
An important question is how to choose frequencies in order to maximize the benefits of EF methods. In this work, we will show that the key to the answer is the analysis of the error's behavior. By following the approach of [2, 3, 4], we develop an algorithm for the estimation of the frequency, by analyzing the behavior of the leading term of the error. Numerical experiments illustrate the obtained results.

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Learning the Hamiltonian of some classes of mechanical systems

Davide Murari (NTNU), Elena Celledoni, Ergys Çokaj, Andrea Leone, Brynjulf Owren

Thu 16:30-17:00 R1.23 Z3

Neural networks have been proven to be effective as a tool for mathematical modelling and model discovery. In this talk, we go through a possible approach to approximate the Hamiltonian of some classes of mechanical systems.

We start from a (large enough) set of measured trajectories coming from a Hamiltonian system X_H, and we want to obtain an approximation of the Hamiltonian H.

The approach we present is based on Recurrent Neural Networks (RNNs), typically used for

time-structured data, as for the trajectories we work with. This framework can be adapted, in principle, to any Hamiltonian system. However, we focus on a class of mechanical systems whose phase space, $T^*Q \subset \mathbb{R}^{2n}$, is a homogeneous manifold. In this setting, we highlight a possible connection between Lie group integrators and this learning framework based on RNNs.

Variational Integrators: high order, multirate dynamics and optimal control
Sina Ober-Blöbaum (University of Paderborn)
Thu 10:50-11:40 R3.07, R3.28 @ Z1

Variational principles are powerful tools for the modelling and simulation of conservative mechanical and electrical systems. As it is well-known, the fulfilment of a variational principle leads to the Euler-Lagrange equations of motion describing the dynamics of such systems. A discretisation of the variational principle leads to unified numerical schemes called variational integrators with powerful structure-preserving properties such as symplecticity, momentum preservation and excellent long-time behaviour.
After a broad introduction to variational integrators we will focus on different recent research aspects. These include high and mixed order construction and convergence analysis of variational integrators, a multirate version for the efficient simulation of dynamics on different time scales as well as their use in solving optimal control problems. The theoretical results will be demonstrated numerically by means of several applications.

Turning an analysis technique into a tool: Identification and simulation of Hamiltonian systems using inverse modified equations
Christian Offen (Paderborn University), Sina Ober-Blöbaum
Tue 11:40-12:05 R3.07 Z1

Hamiltonian systems arise for instance, in classical mechanics, plasma physics, and sampling problems. If a system of ordinary differential equations forms a Hamiltonian system, then the Hamiltonian structure guarantees important qualitative aspects of the dynamical system, such as a lack of attractors, energy conservation, and is related to further topological properties of the phase portrait and conservation laws. Learning Hamiltonian structure from trajectories is an important task in system identification theory. Another challenge is to simulate Hamiltonian dynamics using numerical methods while preserving important structural properties under discretisation. Inverse modified differential equations have recently been introduced as an analysis technique for Hamiltonian neural networks. In this talks I would like to show how to turn this analysis technique into a tool for system identification and structure preserving simulations.

Deep learning as optimal control problems with applications to mechanical systems
Brynjulf Owren (NTNU), Martin Benning, Elena Celledoni, Ergys Cokaj, Matthias Ehrhardt, Christian Etmann, Robert McLachlan, Andrea Leone, Davide Murari, Carola Schönlieb, Ferdia Sherry
Tue 09:00-09:50 R3.07, R3.28 @ Z1

Supervised deep learning can be thought of as a way of approximating an unknown function based on a set of data samples. The space of approximating functions are represented by a neural network. The residual neural networks constitute a particular type of network architecture that enjoys a close connection to ordinary differential equations, the so called neural

ODE. The training of the network can in this sense be cast as a continuous optimal control problem. This allows for a number of opportunities for discretisations and analysis of the resulting dynamical system. We shall discuss some of these features, such as stability and equivariance. In the second part of the talk, we shall present the application of deep neural networks to Hamiltonian systems. We shall then assume that the Hamiltonian is unknown and estimate it from observed measurements by a recurrent neural network. In this case, there will be back propagation on two levels, one for computing the Hamiltonian vector field from the neural network representation of the Hamiltonian, and secondly for computing gradients of the network with respect to the parameters. We consider a hybrid model where the kinetic energy is assumed to have a standard form, whereas the potential energy is represented as a residual neural network. We give some ideas about how to handle constrained Hamiltonian problems. Some numerical experiments will be shown.

Adapted numerical schemes for differential problems

Giovanni Pagano (Department of Mathematics, University of Salerno), Dajana Conte, Beatrice Paternoster

Wed 10:50-11:00 R1.23 Z3

We consider differential problems deriving from applications in real phenomena [1, 2], where some characteristics and properties of the exact solution are a-priori known. Our aim is to develop numerical techniques that are able to preserve such features [3, 4] and that have excellent stability properties [5, 6].
In particular, we will focus on stiff differential problems, whose exact solution is positive and/or oscillates with known frequency. Numerical tests will be shown in order to confirm the efficiency, stability and accuracy of the proposed numerical methods.

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Dual field mass-, energy-, and helicity conserving discretization for the incompressible Navier-Stokes equations

Artur Palha (Delft University of Technology), Yi Zhang, Marc Gerritsma

Thu 16:30-17:00 R3.07 Z1

We introduce a mimetic dual-field discretization which conserves mass, kinetic energy and helicity for three-dimensional incompressible Navier-Stokes equations. The discretization makes use of a conservative dual-field mixed weak formulation where two evolution equations of velocity are employed and dual representations of the solution are sought for each variable. A temporal discretization, which staggers the evolution equations and handles the nonlinearity such that the resulting discrete algebraic systems are linear and decoupled, is constructed. The spatial discretization is mimetic in the sense that the finite dimensional function spaces form a discrete de Rham complex. Conservation of mass, kinetic energy and helicity in the absence of dissipative terms is proven at the discrete level. Proper dissipation rates of kinetic energy and helicity in the viscous case is also proven. Numerical tests supporting the method are provided.

Approximation of SPDE covariance operators by finite elements: A semigroup approach

Andreas Petersson (University of Oslo), Mihály Kovács, Annika Lang

Thu 13:30-14:00 R3.28 Z2

In this talk, we consider the problem of approximating the covariance operator of the mild solution to a linear stochastic partial differential equation (SPDE). An integral equation involving the semigroup of the mild solution is derived and a general error decomposition formula is proven. This formula is applied to approximations of the covariance operator of a stochastic advection-diffusion equation and a stochastic wave equation, both on bounded domains. The approximations are based on finite element discretizations in space and rational approximations of the exponential function in time. Special attention is given to the case that the covariance operator of the underlying Q-Wiener process, which drives the SPDE, has a homogeneous kernel. We derive convergence rates in the trace class and Hilbert–Schmidt norms and we explain how the properties of the kernel of the covariance of the Q-Wiener process affect these rates. Important examples of homogeneous kernels that fit into our framework include the class of Matérn kernels. Numerical simulations illustrate the results.
This presentation is based on joint work with Mihály Kovács and Annika Lang.

A Computational Model of Dengue Transmission by Cellular Automata

Neisser Pino Romero (Universidad Peruana Cayetano Heredia), Gabriel Wainer

Tue 11:40-11:50 R1.23 Z3

In this work, we present a computational model by Cellular Automata (Cell-DEVS) applied to the transmission of Dengue disease, spreads by mosquitoes to a susceptible population. This model has a multilevel approach to consider exogenous interactions such as temperature. It allows to be able to visualize the critical points (infectious foci) where the mosquito reproduction is much greater at high temperatures, in consequence it carries out adequate control strategies.

This disease affects quite a lot the community of the Peruvian jungle as well as the Colombian and Brazilian. Being a problem of collaborative work to prevent an epidemic caused by the mosquito that currently transmits three diseases (dengue, Zika and Chikingunya).

Keys Words: Mathematical Epidemiology. Cellular Automata. DEVS Formalism. Computational Simulations.

Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology

Łukasz Płociniczak (Faculty of Pure and Applied Mathematics, Wroclaw University of Science and Technology)

Tue 13:30-14:10 R3.28 Z2

Many natural and industrial phenomena exhibit nonlocal behaviour in temporal or spatial dimension. The former is responsible for processes for which its whole history influences the present state. The latter, on the other hand, indicates that faraway regions of the domain may have some impact on local points. This is useful in describing media of high heterogeneity.
Partial differential equations that are nonlocal involve one or several integral operators that encode this behaviour. For example, Riemann-Liouville or Caputo derivatives are used in temporal direction, while fractional Laplacian or its relatives describe spatial nonlocality. When it comes to numerical methods the discretization of these requires more care than their classical versions. Moreover, it is usually much more expensive, both on CPU and the memory, to conduct simulations involving nonlocal equations.
In this talk we will present several approaches to discretize nonlocal and nonlinear parabolic equations. These include: transformation into a pure integral equation for the time-fractional porous medium equation and Galerkin spectral methods for a general parabolic equation with temporal nonlocality. We will prove stability and convergence of these methods illustrating all the theoretical results with numerical simulations implemented in Julia programming language with parallelization. The talk is based on [2, 3, 1, 4].

Acknowledgement

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On randomized implicit Runge–Kutta methods

Helmut Podhaisky (Martin Luther University Halle-Wittenberg), Raphael Kruse

Wed 11:30-11:40 R3.28 Z2

Randomized Runge–Kutta methods have been used for the numerical solution of ordinary differential equations with time–irregular coefficient functions, cf. [2, 1]. In the present work we construct a diagonally implicit, A–stable, two-stage scheme which is based on a randomized

trapezoidal quadrature. The method has classical order 2. Numerical experiments with a variable step-size implementation illustrate the convergence properties for a few non-smooth problems.

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On the efficient numerical computation of the matrix Mittag-Leffler function

Marina Popolizio (Politecnico di Bari, Italy), Roberto Garrappa, Tiziano Politi

Tue 14:10-14:50 R3.28 Z2

Important applications in fractional calculus require the numerical computation of the Mittag-Leffler function with matrix arguments. This topic presents sensitive issues that need to be properly addressed. Furthermore, ad hoc numerical strategies are required when large matrices are involved. Numerical methods will be presented, along with numerical tests to demonstrate their effectiveness.

Methods for analysing patterns in solutions of reaction-diffusion equations

Roland Pulch (Universität Greifswald)

Mon 17:05-17:30 R1.23 Z3

We consider reaction-diffusion equations, i.e., a system of partial differential equations (PDEs) in time and two-dimensional space. The equations model the formation of patterns in animal coats and skins, for example. Stationary solutions represent a final pattern, which depends both on physical parameters and initial values. A spatial finite difference method yields a high-dimensional system of ordinary differential equations (ODEs). Stationary solutions of the ODEs are computed to approximate steady-state solutions of the PDEs.

We investigate properties of the patterns using methods from image processing. The two-dimensional stationary solutions are converted into binary images. This approach allows for the application of morphological operations on the binary image. Euler numbers and Feret diameters can be determined, for example. Moreover, we examine associated statistical quantities for sample sets of initial values in a Monte-Carlo simulation. Our aim is to analyse the dependence as well as the sensitivity of patterns on the parameters. We present results of numerical computations for different selections of those parameters.

The geometry of embeddings

Philipp Reiter (Chemnitz University of Technology), Sören Bartels, Henrik Schumacher

Mon 14:00-14:25 R1.23 Z3

In pursuit of finding "optimal" embeddings of curves and surfaces with prescribed topology, one may study repulsive functionals such as the tangent-point potential. Analytical and numerical challenges result from the highly nonlinear and nonlocal nature of these objects.
Local minimizers can be approximated by considering various gradient flows. The choice of an appropriate metric is crucial both for performance and stability.
In this talk I will outline some recent results which will be illustrated by a few numerical examples.

A posteriori error estimation for Physics Inspired Neural Network solutions to partial differential equations

Thomas Richter (Otto-von-Guericke Universität Magdeburg), Piotr Minakowski

Tue 18:00-18:30 R3.07 Z1

We present an a posteriori error estimator for solutions of partial differential equations represented with neural networks. We have in mind the different variants of Physics Informed Neural Networks, e.g. the *Deep Ritz* method of E and Yu or the *Deep XDE* approach according to Lu, Meng, Mao and Karniadakis.
The error estimator is based on dual solutions and can estimate errors in general objective functionals, e.g. point evaluation of the solution. We show the ease of implementation and high accuracy of the method. Besides measuring the actual error of the neural network solution, another possible application is to serve as stopping criterion while training the neural network.

Reduced order methods: state of the art, perspectives and applications in computational fluid dynamics

Gianluigi Rozza (SISSA, Int. School for Advanced Studies, Trieste)

Tue 08:10-09:00 R3.07, R3.28 @ Z1

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: a better use of stable high fidelity methods, considering also spectral element method and finite volume discretisations, to enhance the quality of the reduced model too, and allowing to incorporate some turbulent patterns and increasing the Reynolds number; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, as well as the dimension of online systems; 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. For nonlinear systems, also the investigation on bifurcations of parametric solutions are crucial and they may be obtained thanks to a reduced eigenvalue analysis of the linearised operator. All the previous aspects are very important in CFD problems to focus in real time on complex parametric industrial, environmental and biomedical flow problems, or even in a control flow setting with data assimilation or uncertainty quantification. Model flow problems will focus on few benchmarks, as well as on simple fluid-structure interaction problems and shape optimisation applied to industrial problems.

A pair of two-step hybrid block methods using a variable stepsize formulation for integrating third-order Lane-Emden-Fowler equations.

Mufutau Rufai (University of Bari, Aldo Moro), Higinio Ramos

Wed 11:30-11:40 R1.23 Z3

In this talk, a variable step-size formulation of a pair of two-step hybrid block methods will be proposed and efficiently applied for integrating linear and nonlinear third-order Lane-Emden-Fowler model equations using large integration intervals. The basic properties of the new schemes will be theoretically analysed. The proposed methods will be implemented in an adaptive mode by adapting the number and position of the nodes utilised in the approximation to assure that the truncation error is kept and saved within a specified bound. The reliable and accurate performance shall be observed for the introduced methods based on reasonable error estimation and adaptive strategy presented in this talk. Finally, some models third-order Lane-Emden-Fowler problems will be numerically solved to assess the performance and efficiency of the proposed techniques.

Numerical simulation of stochastic evolution equations with non-commutative noise

Andreas Rößler (Universität zu Lübeck, Institute of Mathematics), Claudine von Hallern

Thu 14:00-14:30 R3.28 Z2

We consider the problem of approximating mild solutions of stochastic evolution equations in the mean-square sense. Therefore, an infinite dimensional version of a Runge-Kutta type scheme for the time discretization is proposed. The introduced scheme can be applied to a certain class of semilinear stochastic partial differential equations (SPDEs) with commutative as well as non-commutative noise. In case of non-commutative noise, iterated stochastic integrals of the driving Q-Wiener process have to approximated. Finally, the order of convergence and the efficiency of the new scheme will be discussed.
This is joint work with Claudine von Hallern (Universität Hamburg)

Investigation of the role of frictional contact interactions in the mechanical response of spiral strands using 1D finite strain beam model

Mohammad Ali Saadat (CentraleSupélec), Damien Durville

Tue 16:30-17:00 R1.23 Z3

In this study, the role of frictional contact interactions in the mechanical behavior of spiral strands is investigated. To this end, the wires have been modeled using 1D finite strain beam model with point-wise frictional contact interactions. It is shown that the frictional contact interaction does not play a significant role in the tensile response of the strand, while this is not the case for bending. It is well known that the interwire frictional contact causes a nonlinear bending behavior for spiral strands. In order to explain the experimental results, in which the spiral strands exhibit very high bending stiffness without any external tensile force, the presence of residual stresses due to manufacturing process is suggested. Due to the unknown state of residual stresses, the effect of these stresses has been considered by a simple method.

High-order integrators on homogeneous spaces via nonholonomic mechanics
Rodrigo T. Sato Martín de Almagro (FAU - Lehrstuhl für Technische Dynamik)
Thu 14:30-15:00 R1.23 Z3

In this talk, high-order numerical integrators on homogeneous spaces will be presented as an application of nonholonomic partitioned RKMK methods on Lie groups.

A homogeneous space M is a manifold where a group G acts transitively. Such a space can be understood as a quotient $M \cong G/H$, where H a closed Lie subgroup, is the isotropy group of each point of M. The Lie algebra of G decomposes into $\mathfrak{g} = \mathfrak{m} \oplus \mathfrak{h}$, where $\mathfrak{h}$ is the subalgebra associated with H. Thus, variational problems on M can be treated as nonholonomically constrained problems on G, by requiring variations to remain on $\mathfrak{m}$.

Nonholonomic partitioned RKMK integrators are derived as a modification of those obtained by a discrete variational principle on Lie groups, and can be interpreted as obeying a discrete Chetaev principle. These integrators seem to preserve several properties of their purely variational counterparts.

Optimal control of gas network DAEs
Henning Sauter (HU Berlin), Caren Tischendorf
Mon 14:50-15:15 R3.28 Z2

The physics in a gas flow network can be described by the Euler equations. In case that the temperature of the gas is assumed to be constant, a simplified model (ISO-2) can be derived. Additional algebraic restrictions such as bounds on the pressure and flow can be added yielding an overdetermined PDAE system. While the efficient and accurate simulation of the network is interesting in its own right, a more challenging aspect is to consider optimal control problems on these networks.
Typically, these problems are solved using either a *discretize-then-optimize* or an *optimize-then-discretize* approach. We demonstrate a novel approach consisting of 1. *discretize-in-space*, 2. *optimize*, 3. *discretize-in-time*. Firstly, a suitable spatial discretization scheme is used resulting in a DAE system of the network. Subsequently, we use an adjoint calculus approach to obtain the *optimality DAE*, which is then in turn discretized in time to obtain a solution both for the network state and the optimal control.
We demonstrate the procedure, comment on the connection of the optimal control problem and the optimality DAE and show a few numerical results.

Numerical modeling for stochastic oscillators
Carmela Scalone (University of L'Aquila), Raffaele D'Ambrosio
Wed 10:50-11:00 R3.28 Z2

Scientific literature provides several models describing the dynamics of different types of oscillators, both in deterministic and stochastic setting. The majority of the examples of stochastic oscillator are obtained by introducing a *noisy ingredient* in an underlying deterministic model. This noisy component may be an additive and/ or a multiplicative noise, a random frequency, a random damping, and so on (see [1] and references therein for a survey). A numerical issue tipically investigated in this setting is the attitude of classical numerical schemes for SDEs to preserve of long term properties of particular oscillators, see [2]. The variety of models inspires the construction of specific methods to solve particular stochastic equations, which describe oscillatory dynamics, see [3]. We present our results in terms of a study of conservation, see [4], and of providing targeted methods for very popular examples of oscillators, see [5, 6].

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Monotone SPDEs with Algebraic Constraints

Maximilian Schade (Humboldt-Universität zu Berlin), Caren Tischendorf, Nicolas Perkowski

Thu 16:00-16:30 R3.28 Z2

This talk is about a new stochastic framework for solving energy networks arising in circuit simulation and gas transport. Particular foci are the uncertainties caused by fluctuations in demand and supply. Neglecting these uncertainties, the transient behavior of such networks can be described by systems of partial differential equations (e.g. the Euler equations for gas networks) coupled via algebraic constraints. Here, we study an approach using a semi-explicit prototype for the coupling of algebraic equations with an SDE and an SPDE. We take a look at existing theory and extend this to our prototype to get existence and uniqueness under specific assumptions. Considering energy networks, we discuss how restrictive these assumptions are by taking a closer look at circuit simulation and gas transport in this stochastic setting.

Resonances as a computational tool

Katharina Schratz (Sorbonne University)

Thu 08:10-09:00 R3.07, R3.28 @ Z1

Linear problems and smooth solutions are nowadays well understood, a reliable description of 'non-smooth' phenomena remains one of the most challenging open problems in computational mathematics. Nevertheless, 'non-smooth phenomena' play a fundamental role in modern physical modeling (e.g., blow-up phenomena, turbulences, high frequencies, low dispersion limits, etc.) which makes it an essential task to find suitable numerical schemes. In this talk I present a new class of low regularity integrators. The key idea in the construction of the new schemes lies in embedding the underlying oscillatory structure of the PDE into the numerical discretisation, addressing the fundamental question: How and to what extent can we reproduce the qualitative behavior of partial differential equations in a finite (discretized) world?

Cauchy Contour Integration based REXI methods for Climate and Weather simulations

Martin Schreiber (Université Grenoble Alpes, Jean Kuntzmann Laboratory, AIRSEA team), Jed Brown

Thu 17:00-17:30 R3.07 Z1

Running simulations on high-performance computers poses restrictions and therefore challenges on solving PDEs within a particular time frame. Here, disruptive mathematical reformulations which, e.g., exploit additional degrees of parallelism also in the time dimension gained increasing interest over the last two decades.
This talk targets improving the wallclock time for weather and climate simulations and starts by giving a brief overview of exponential integration methods. Then, the focus is put on rational approximations of exponential integrating (REXI) methods and its successful application to prototypes of single-layer atmospheric simulations. We will present our current work on Gaussian-quadrature Cauchy Contour integration methods and compare it to other state-of-the art time integration methods which can be posed in the REXI form (B-REXI, T-REXI, EL-REXI, CI-REXI).
(I gratefully acknowledge contributions, discussions and more with Jed Brown, Finn Capelle, Terry S. Haut, Pedro S. Peixoto and Raphael Schilling)

Advanced Newton methods for geodynamical models of Stokes flow with viscoplastic rheologies

Yu-hsuan Shih (New York University), Georg Stadler, Johann Rudi

Thu 17:30-18:00 R3.07 Z1

Stokes equations with viscoplastic rheologies play an important role in geodynamics. The nonlinearities of these rheologies make the numerical solution of the resulting systems challenging, and iterative methods often converge slowly or not at all. Yet accurate solutions are critical for representing the physics. We study a basic but representative viscoplastic rheology law which involves a yield stress that is independent of the dynamic pressure, referred to as von Mises yield criterion. We propose a new stress–velocity Newton solution algorithm that treats the stress as an independent variable during the Newton linearization but requires solution only of Stokes systems that are of the usual velocity–pressure form. Comparing the performance of the proposed Newton method with the standard Newton method and the Picard fixed-point method, we observe a significant reduction in the number of iterations and improved stability with respect to problem nonlinearity, mesh refinement, and the polynomial order of the discretization.

Compatible finite elements and parallel-in-time schemes for geophysical fluid dynamics

Jemma Shipton (University of Exeter), Colin Cotter, Thomas Bendall, Thomas Gibson, Lawrence Mitchell, David Ham, Beth Wingate, Dave Acreman, Omar Jamil, Owen Rowell

Thu 13:30-14:00 R3.07 Z1

I will describe Gusto, a dynamical core toolkit built on top of the Firedrake finite element library; present recent results from a range of test cases and outline our plans for the development of time-parallel algorithms.
Gusto uses compatible finite element methods, a form of mixed finite element method (meaning that different finite element spaces are used for different fields) that allow the exact representation of the standard vector calculus identities div-curl=0 and curl-grad=0. The popularity of

these methods for numerical weather prediction is due to the flexibility to run on non-orthogonal grids, thus avoiding the communication bottleneck at the poles, while retaining the necessary convergence and wave propagation properties required for accuracy.
Although the flexibility of the compatible finite element spatial discretisation improves the parallel scalability of the model, it does not solve the parallel scalability problem inherent in the sequential timestepping: we need to find a way to perform parallel computations in the time domain. Exponential integrators, approximated by a near-optimal rational expansion, offer a way to take large timesteps and form the basis for parallel timestepping schemes based on wave averaging. I will describe the progress we have made towards implementing these schemes in Gusto.

Convergence acceleration of heterogeneous domain decomposition method for EMT-TS electrical network DAE system.

Héléna Shourick (SuperGrid Institute, Université Claude Bernard Lyon 1, Institut Camille Jordan), Damien Tromeur-Dervout, Laurent Chedot
Mon 15:15-15:40 R3.28 Z2

Simulation of power grid consists in solving a system of differential algebraic equations (DAE) where the unknowns are currents and voltages. The Modified Augmented Nodal Analysis allows us to build the DAE system where each component of the grid contributes through relations between currents and voltages and the Kirshoff's laws give the algebraic constraints. The introduction of power electronic components implies faster dynamics than before. Therefore, as some areas of the network require a high level of detail in the simulation as well as the ability to model faster dynamics, they are modeled by Electromagnetic Transient (EMT) modeling type, while the rest of the network is modeled using a more computationally efficient type of modeling: dynamic phasor model (TS). These two types of modeling lead to adapted DAE subsystems. To co-simulate these two subsystems, which involve different time steps, we use an overlapping Schwarz heterogeneous domain decomposition method (DDM) to exchange transmission conditions between models. We examine the influence of the cutting location on the method, as well as the influence of two different models (EMT-TS) on the information to be exchanged. We show on a linear electric circuit the convergence property of the DDM with and without overlap and use the pure linear divergence of the method to accelerate it towards the solution with the Aitken's acceleration technique.

Numerical simulations of dead zone formation in the catalytic flow-through membrane reactor

Piotr Skrzypacz (School of Sciences and Humanities, Nazarbayev University), Nagima Chalkarova; Boris Golman; Vsevolod Andreev; Friedhelm Schieweck; Kuralay Tilegen
Wed 11:00-11:10 R3.07 Z1

The use of catalytic membranes in chemical reactor engineering has significantly improved the reactor performance. Therefore, mathematical modelling and numerical simulations of catalytic membrane reactors are important for optimal parameter design increasing the selectivity and yield of certain products in chemical reactions. In this talk, the mathematical model of the flow-through catalytic membrane reactor is presented. The model is based on coupled nonlinear convection-diffusion-reaction equations with temperature-dependent reaction rate constants. The series reactions in the reactor are characterized by the power-law kinetics of fractional order which until now has been rarely investigated in the literature. Under specific reaction and process conditions the reactant can be depleted and a dead-zone can be formed in the

membrane reactor. The numerical simulation of this phenomenon requires special solvers. The key idea in this presentation is to construct an appropriate time-marching scheme for solving the steady-state model equations. The effects of parameters such as reaction order, Peclet number, and Thiele modulus on solution profiles and formation of dead-zones are studied numerically. The simulation results show how these parameters influence the appearance and size of the dead zone for the non-isothermal multi-reaction systems.

Structure-preserving hybrid methods

Ari Stern (Washington University in St. Louis)

Fri 11:40-12:30 R3.07, R3.28 @ Z1

The classical finite element method uses piecewise-polynomial function spaces satisfying continuity and boundary conditions. Hybrid finite element methods, by contrast, drop these continuity and boundary conditions from the function spaces and instead enforce them weakly using Lagrange multipliers. The hybrid approach has several numerical and implementational advantages, which have been studied over the last few decades.
In this talk, we show how this hybrid framework has given new insight into a variety of structure-preserving methods for differential equations, including (multi)symplectic methods for Hamiltonian systems, charge-conserving methods for the Maxwell and Yang-Mills equations, and finite element exterior calculus. In particular, this provides a bridge linking geometric numerical integration of ODEs to numerical PDEs.

Convergence Criteria for Co-Simulation of Coupled Network DAEs

Caren Tischendorf (Humboldt-Universität zu Berlin), Jonas Pade

Mon 14:00-14:25 R3.28 Z2

First, we present a general convergence result for a co-simulation of Gauß-Seidel and of Jacobi type for coupled DAEs of the form

$$f_1(\frac{\mathrm{d}}{\mathrm{d}t}m_1(x_1,t), x_1, g_2(x_2), t) = 0,$$
$$f_2(\frac{\mathrm{d}}{\mathrm{d}t}m_2(x_2,t), x_2, g_1(x_1), t) = 0.$$

Both DAEs may have a higher index but the perturbation index of the systems

$$f_i(\frac{\mathrm{d}}{\mathrm{d}t}m_i(x_i,t), x_i, \delta_i, t) = 0$$

is assumed to be not larger than 1 for perturbations δ_i and $i \in \{1,2\}$. Note that the perturbations δ_i reflect only perturbations at the interface between both DAE systems. We demonstrate how the convergence rate can be influenced by the interplay of the interface functions g_1 and g_2 with the DAE model functions f_1 and f_2.
In the second part, we discuss particular DAE models for flow networks (circuits, energy systems, networks of neurons) and provide network topological convergence criteria for the co-simulation.

On the exact tangent matrices of a geometrically exact beam formulated on the special Euclidean group SE(3)

Juliano Todesco (Aerospace and Mechanics Engineering Department(LTAS), University of Liège), Olivier Brüls

Tue 14:00-14:30 R1.23 Z3

This work presents the exact tangent matrices of a geometrically exact beam finite element formulated on the special Euclidean group SE(3)[1]. The objective is to obtain optimal convergence of Newton-Raphson iterations with an implicit time integration procedure and allow the semi-analytic calculation of the sensitivity of flexible multibody systems for optimization purposes.

A beam is a structural element having one of its dimensions much larger than the other two. The neutral axis corresponds to the beam's centerline, defined along that longer dimension and its cross-sectional plane, which is normal to the long axis. At any point of the centerline, the cross-section position and orientation are represented by a local frame. Each local frame has 6 degrees of freedom, namely three translations and three rotations. The transformation between the inertial and the local frame is represented by an element on the special Euclidean group SE (3). The beam is represented on the special Euclidean group SE(3) using a motion approach; hence, the position and rotation fields are treated as a unit. The geometric description of the element is based on the representation of the frame transformation as 4×4 homogeneous transformation matrices $\mathbf{H}$.

$$\mathbf{H} = \begin{bmatrix} \mathbf{R} & \mathbf{x} \\ \mathbf{0}_{1\times 3} & 1 \end{bmatrix}$$

where $\mathbf{x}$ is a 3×1 vector defining the position of the local frame and $\mathbf{R}$ is a 3×3 rotation matrix defining the orientation of the local frame. In order to express the local frames along the beam's reference curve, a two-node element is used. The finite element interpolation of the local frame is based on the exponential map of the special Euclidean group SE(3), a non-commutative and non-linear space. This finite element discretization procedure generates helicoidal shape functions.

The coupling between rotation and translation introduced by these the helicoidal functions yields a naturally locking-free element that can efficiently capture non-linear deformation patterns of elastic beams. For instance, when applied to a pure bending/torsion case, a single element can be used and the exact solution achieved. The equations of motion generated from this approach take the form of second-order differential-algebraic equations on a Lie group; they are solved using a Lie group time integration scheme, namely, the generalized-α method proposed by Brüls et al [2].

The non-linear set of equations and the iterative Newton-Raphson time integration require that the tangent matrices must be computed at each iteration. Indeed, the more accurate the tangent matrices are calculated, the less is the possibility of divergence and the number of iterations needed to reach the desired numerical tolerance. It has an advantage when extremely bent/twisted beams need to be captured while employing relatively coarse meshes and large time steps. Therefore, in order to achieve higher accuracy, the exact tangent matrices, in other words, all the terms in the linearized equation of motion, have to be considered; these terms were entirely derived herein. This has been hardly addressed in the literature. In addition, exact tangent matrices are mandatory for semi-analytic calculation of the sensitivity analysis of both the adjoint variable and direct differentiation methods[3].

Moreover, numerical and implementation issues related to truncation errors, the range of applicability and singularity were addressed and explored. The exponential map and its tangent operator have two options to be calculated. The first option is an infinite serial expansion; hence, it must be truncated to a finite number of terms. Consequently, it has a truncation

error. However, the truncation error decreases as it approaches the origin of the exponential map of the SE(3). The second option is the serial expansion's close-form which is an expression composed of trigonometric terms. However, it suffers from a singularity at the origin. Thus, the error increases approaching the origin. Regarding the tangent matrices, it uses the tangent operator and its directional derivatives. In previous studies, the directional derivatives have been essentially computed using trigonometric close-form. To circumvent singularity and accuracy issues typical of the trigonometric approach, we proposed an approach based on an expansion series; this has the advantage of high precision close to the origin, and it is free of singularity at the origin.
Two numerical tests were performed to assess the approach developed here. The first test showed a relative error of the tangent operator and its directional derivatives considering both the series and close-form expressions. Therefore, it allowed the development of a strategy to control the numerical error according to the desired tolerance. The results indicated that a switch between the series and close-form expressions for the tangent operator and its directional derivatives in the range $[0, \pi]$ is recommended to guarantee high accuracy and cost-effective computations. The second numerical test assured that the exact tangent matrix was obtained for the geometrically exact beam formulated on the special Euclidean group SE(3). The error analyses were compared against the finite-difference method, and the results indicated that the exact matrix was obtained by using the methods developed here.
The exact tangent matrices developed here, the numerical strategies and the tests performed have attested that an optimal convergence can be obtained using the iterative Newton-Raphson method. The approaches developed were further explored using detailed sensitivity analyses. The methods developed here proved to be robust, cost-effective and appropriate to be applied on flexible multibody systems where optimization techniques are crucial.
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Schwarz and Schur time domain decomposition for nonlinear ODE

Damien Tromeur-Dervout (Université de Lyon, Institut Camille Jordan
UMR5208-CNRS-U.Lyon1)

Mon 17:05-17:30 R3.07 Z1

We developed parallel time domain decomposition methods to solve systems of linear ordinary differential equations (ODEs) based on the Aitken-Schwarz [5, 3] or primal Schur complement domain decomposition methods [2]. The methods require the transformation of the initial value problem in time defined on $]0, T]$ into a time boundary values problem. Let $f(t, y(t))$ be a function belonging to $\mathcal{C}^1(\mathbb{R}^+, \mathbb{R}^d)$ and consider the Cauchy problem for the first order ODE:

$$\left\{\dot{y} = f(t, y(t)),\ t \in]0, T],\ y(0) = \alpha \in \mathbb{R}^d. \right. \tag{1}$$

The time interval $[0, T]$ is split into p time slices $S^{(i)} = [T_{i-1}^+, T_i^-]$, with $T_0^+ = 0$ and $T_p^- = T^-$. The difficulty is to match the solutions $y_i(t)$ defined on $S^{(i)}$ at the boundaries T_{i-1}^+ and T_i^-. Most of time domain decomposition methods are shooting methods [1] where the jumps $y_i(T_i^-) - y_{i+1}(T_i^+)$ are corrected by a sequential process which is propagated in the forward direction (i.e. the correction on the time slice $S^{(i-1)}$ is needed to compute the correction on

time slice $S^{(i)}$). Our approach consists in breaking the sequentiality of the update of each time slice initial value. To this end, we transform the initial value problem (IVP) into a boundary values problem (BVP) leading to a second order ODE:

$$\begin{cases} \ddot{y}(t) = g(t, y(t), \dot{y}(t)) \stackrel{def}{=} \dfrac{\partial f}{\partial t}(t, y(t)) + \dot{y}(t)\dfrac{\partial f}{\partial y}(t, y(t)),\ t \in]0, T[, & \text{(2a)} \\ y(0) = \alpha, & \text{(2b)} \\ \dot{y}(T) = \beta \stackrel{def}{=} f(T, y(T)) & \text{(2c)} \end{cases}$$

Then classical domain decomposition methods apply such as the multiplicative Schwarz method with no overlapping time slices and Dirichlet-Neumann transmission conditions (T.C.) for linear system of ODE (or PDE [4]). As proved in [3] the convergence/divergence of the error at the boundaries of this Schwarz time DDM can be accelerated by the Aitken technique to the right solution when $f(t, y(t))$ is linear. Nevertheless, the difficulty in solving equation (2) is that β is not given by the original IVP. In this talk, we investigate the proposed approach for nonlinear ODE.

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Numerical investigation of stability of coarse grid discretisations for dissipative systems

Denise Tumiotto (Martin-Luther-Universität Halle-Wittenberg), Martin Arnold

Thu 13:00-13:30 R1.23 Z3

Numeric methods of Newmark family are well known and largely used when solving stiff problems, [2]. Some examples include the Newmark-β, the HHT-α method, and the generalized-α [1]. The latter is of much interest because of its unconditional stability and second order convergence, proved only for linear problems. Moreover, the generalized-α scheme has optimal user-defined numerical dissipation.

Another family of numerical integrators is the family of variational integrators [3]. In particular, the present work introduces as an example the implicit midpoint rule. The implicit midpoint rule is a symplectic method with second order convergence.

Introducing the dissipation in the formulation of the system, we obtain a nonlinear dissipative system. We investigate the stability of the numerical methods for the resulting system. In order to perform the study, we introduce the model of an elastic pendulum in two different configurations: the floating frame of reference, [4], and the finite segment. The analysis proceeds through the comparison in the energy trend both for conservative and dissipative systems.

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Stochastic variational principles for the collisional Vlasov-Maxwell and Vlasov-Poisson equations

Tomasz Tyranowski (Max Planck Institute for Plasma Physics)

Thu 14:30-15:00 R3.07 Z1

In this work we recast the collisional Vlasov-Maxwell and Vlasov-Poisson equations as systems of coupled stochastic and partial differential equations, and we derive stochastic variational principles which underlie such reformulations. We also propose a stochastic particle method for the collisional Vlasov-Maxwell equations and provide a variational characterization of it, which can be used as a basis for a further development of stochastic structure-preserving particle-in-cell integrators.

Superconvergent methods inspired by the Crank-Nicolson scheme in the context of diffusion PDEs (deterministic and stochastic)

Gilles Vilmart (University of Geneva), based on joint works with Assyr Abdulle, Ibrahim Almuslimani, Guillaume Bertoli, Christophe Besse, and Charles-Edouard Bréhier

Fri 09:00-09:50 R3.07, R3.28 @ Z1

In this talk, we present two different situations where the Crank-Nicolson method is surprisingly more accurate than one could expect and inspires the design of new efficient numerical integrators:

- **in the context of splitting methods for parabolic PDEs [3, 4]:** we show that the Strang splitting method applied to a diffusion-reaction equation with inhomogeneous general oblique boundary conditions is of order two when the diffusion equation is solved with the Crank-Nicolson method, while order reduction occurs in general if using other

Runge-Kutta schemes or even the exact flow itself for the diffusion part. We prove [4] these results when the source term only depends on the space variable, an assumption which makes the splitting scheme equivalent to the Crank-Nicolson method itself applied to the whole problem.

- **in the context of ergodic parabolic stochastic PDEs [5, 1, 2]:** although the Crank-Nicolson method can sample exactly the invariant measure of ergodic stochastic differential equations in the Gaussian case, it is only A-stable and lacks the L-stability property which is desirable for a fast convergence to equilibrium. Using the idea of post-processing, we investigate how the L-stability property and the exactness for the invariant measure in the Gaussian case can be achieved simultaneously. We present such schemes applied to nonlinear ergodic problems in the context of implicit Runge-Kutta methods [5] and in the context of explicit stabilized Runge-Kutta methods [1], which can be shown to be strongly convergent [2] for a class of quasilinear parabolic stochastic PDEs, including the quasilinear stochastic heat equation with space-time white noise.

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Multirate Training of Neural Networks

Tiffany Vlaar (University of Edinburgh), Benedict Leimkuhler

Tue 17:30-18:00 R3.07 Z1

We propose multirate training of neural networks: partitioning neural network parameters into fast and slow parts which are trained simultaneously using different learning rates. By choosing appropriate partitionings we can obtain large computational speed-ups for transfer learning tasks. We show that for various transfer learning applications in vision and NLP we can fine-tune deep neural networks in almost half the time, without reducing the generalization performance of the resulting model. We also discuss other splitting choices for the neural network parameters which are beneficial in enhancing generalization performance in settings where neural networks are trained from scratch. Finally, we propose an additional multirate technique which can learn different features present in the data by training the full network on different time scales simultaneously. The benefits of using this approach are illustrated for ResNet architectures on image data. Our paper unlocks the potential of using multirate techniques for neural network training and provides many starting points for future work in this area.

Modeling the interatomic potential by deep learning

Han Wang (Institute of Applied Physics and Computational Mathematics)

Tue 14:30-15:00 R3.07 Z1

In silico design of materials requires an accurate description of the interatomic potential energy surface (PES). However, in the context of molecular simulation, one usually faces the dilemma that the first principle PESs are accurate but computationally expensive, while the empirical PESs (force fields) are efficient but of limited accuracy. We discuss the solution in two aspects: PES construction and data generation. In terms of PES construction, we introduce the Deep Potential (DP) method, which faithfully represents the first principles PESs by a symmetry-preserving deep neural network. In terms of data generation, we present a concurrent learning scheme named Deep Potential Generator (DP-GEN). This approach automatically generates the most compact training dataset that enables the training of DP with uniform accuracy. In the last part of the talk, we present the attempt of implementation and optimization of DP on a heterogeneous high-performance supercomputer Summit, by which one can simulate more than 1 nanosecond-long molecular dynamics trajectory of over 100 million atoms per day.

Implicit Euler Scheme for Stochastic Partial Differential Equations with Monotone Drift

Johanna Weinberger (Institut für Mathematik, Martin-Luther-Universität Halle-Wittenberg)

Tue 11:15-11:40 R3.28 Z2

In this talk we derive convergence rates for the implicit Euler scheme for stochastic partial differential equations (SPDE). Using the variational formulation of the SPDEs according to E. Pardoux, N. Krylov et al. (1972) allows us to consider nonlinear problems like the stochastic p-Laplace equation. For the time stepping analysis we use techniques developed by R.H. Nochetto, G. Savaré, C. Verdi for deterministic evolution equations and combine them with the appraoch from the time stepping analysis of multi-valued SODEs from M. Eisenmann, M. Kovacs, R. Kruse and S. Larsson. Furthermore, we apply the Galerkin method to arrive at a fully discrete scheme.

The BDF2-Maruyama Method for Stochastic Evolution Equations with Monotone Non-Lipschitz Drift

Rico Weiske (Martin-Luther-University Halle-Wittenberg), Raphael Kruse

Thu 16:30-17:00 R3.28 Z2

We investigate the numerical approximation of stochastic evolution equations whose drift operators satisfy a monotonicity condition and are locally Lipschitz continuous. For the underlying numerical method, we utilize the two-step backward difference formula (BDF2) for the time discretization in conjunction with an abstract Galerkin scheme.
In the talk, we establish for the BDF2-Maruyama method a rate of convergence in the strong sense by using the variational approach. The error analysis is based on the concept of p-variation to measure the temporal regularity of the analytical solution. To illustrate our result, we discuss how the stochastic Allen–Cahn equation fits into our framework.
This is joint work with Raphael Kruse (MLU Halle–Wittenberg).

SRKCD: a stabilized Runge-Kutta method for large-scale optimization problems
Måns Williamson (Lund University), Tony Stillfjord
Wed 11:20-11:30 R3.28 Z2

In large-scale machine learning problems, one typically faces the problem of finding the minimum of a loss function which depends on many parameters of large dimensionality. Because of this, standard optimization algorithms such as the gradient descent are often too costly to be used. The classic, popular solution to this is to use an algorithm known as the stochastic gradient descent. This can be described as a version of the traditional gradient descent where each update depends on a random parameter. However, by reformulating the problem as a gradient flow, we see that gradient descent is equivalent to the explicit Euler time-stepping scheme, which has a very small stability region. For many problems, this prevents us from taking large steps and reaching the minimum quickly. This is an issue also for the stochastic version.
In this talk, we consider instead the Runge–Kutta–Chebyshev algorithms, which are explicit time integration methods designed such that their stability region are maximized. It has recently been shown that these methods perform very well in the deterministic optimization setting, i.e. for full gradient descent, with supporting theory for convex quadratic problems. Here, we extend this to the stochastic case. We prove convergence in expectation to a unique minimum for strongly convex, nonlinear functions. A similar approach also leads to convergence for non-convex functions, but in a weaker sense. Finally, we consider a numerical example arising from a supervised learning application which demonstrates the benefits of the scheme.

A generalized midpoint-based boundary-value method for unstable PDEs
Paul Andries Zegeling (Utrecht University), Max van Spengler
Tue 10:50-11:15 R3.07 Z1

We present a boundary-value method (BVM) that can be used for partial differential equation (PDE) models having semi-stable, unstable or even ill-posed, properties. Traditionally, step-by-step methods, such as Runge-Kutta and linear multistep methods, are used for time-dependent models. However, their numerical stability regions (this holds for all explicit and implicit methods) are such that a significant part does not intersect with areas in the complex plane which are of importance for a stable time-integration of unstable DEs. BVMs, that need extra numerical conditions at the final time, are global methods and are, in some sense, free of such barriers. As an example, BVMs based on generalized midpoint methods combined with appropriate numerical initial and final conditions, possess the whole complex plane (excluding the imaginary axis) as stability region. On the other hand, obviously they loose some efficiency, since an extended linear or nonlinear system has to be solved for the whole time range of interest. We will illustrate the usefulness of such methods for several PDE models, such as a dispersive wave equation, a space-fractional PDE and the backward heat equation.

SympNets & PNNs: Intrinsic structure-preserving networks for identifying Hamiltonian & Poisson systems
Zhen Zhang (Brown University), Pengzhan Jin, Yannis Kevrekidis, George Karniadakis
Tue 16:30-17:00 R3.07 Z1

This talk is about new machine learning tools Symplectic networks (SympNets) and Poisson neural networks (PNNs) which can learn Hamiltonian/Poisson systems from data. We prove the universal approximation theorems of both neural networks within the class of symplectic/Poisson map. We showed that any symplectic/Poisson map can be approximately factorized into

unit triangular matrix-like maps in a simple form, i.e. SympNets/PNNs. Simulation results shows that by incorporating prior knowledge into the neural networks, even very small size SympNets/PNNs can generalize well, and are able to handle both Hamiltonian/Poisson systems with data points resulting from short or long time steps.

Bulk-surface Lie splitting for parabolic problems with dynamic boundary conditions

Christoph Zimmer (Universität Augsburg), Robert Altmann, Balázs Kovács

Wed 11:10-11:20 R3.07 Z1

This talk studies a novel bulk–surface splitting method of first order for (semi-linear) parabolic partial differential equations with dynamic boundary conditions, e.g., systems of the form

$$\begin{aligned} \dot{u} - \nabla \cdot (\nabla u) &= f_\Omega(u) \qquad \text{in } \Omega, \\ \dot{u} - \beta\, \Delta_\Gamma u + n \cdot \nabla u + u &= f_\Gamma(u) \qquad \text{on } \Gamma \end{aligned}$$

with $\beta \geq 0$. In general, dynamic boundary conditions appear in applications where the momentum on the boundary should not be neglected, like in models of heat sources on the boundary.
The proposed Lie splitting scheme is based on considering the boundary conditions as a second dynamical system, which is coupled to the bulk problem. The splitting approach is combined with bulk–surface finite elements and an implicit Euler discretization of the subsystems. While other known first-order splittings schemes technically do not approximate the spatially discretized system, our proposed scheme converges to the expect one at the cost of a weak coupling condition of the form $\tau \lesssim h$. The convergence is illustrated also numerically.

BAMPHI (Backward-accurate Action of Matrix PHI-functions)

Franco Zivcovich (Sorbonne Université), Marco Caliari, Fabio Cassini

Mon 15:15-15:40 R3.07 Z1

The time integration of stiff systems of differential equations as

$$u'(t) = F(t, u(t)), \quad u(0) = u_0,$$

constitutes a heated topic in numerical analysis. In particular, exponential integrators drew a great deal of attention. In fact, similarly to implicit methods, these methods show good stability properties, allowing integration with large time steps. Each exponential integration step of length τ (out of hundreds, thousands or even millions steps) consists of the same operation: let $\mathbf{A}$ be the linear part of $F(t, u(t))$ (or, say, its Jacobian), one shall compute

$$u^{n+1} := \varphi_0(\theta_0 \tau \mathbf{A}) v_0 + \varphi_1(\theta_1 \tau \mathbf{A}) v_1 + \ldots + \varphi_p(\theta_p \tau \mathbf{A}) v_p,$$

where $\theta_0, \theta_1, \ldots, \theta_p$ are fixed scalars,

$$\varphi_\ell(x) := \sum_{j=0}^{\infty} \frac{x^j}{(j+\ell)!}, \quad \ell = 0, 1, \ldots, p$$

and the vectors $v_0, v_1, \ldots, v_p \in \mathbb{C}^N$ are obtained, in a recursive fashion, as functions of linear combinations of φ–functions applied to vectors connected to the current state of the system u^n. The authors exploited this peculiarity of exponential integrators and recent advancements in numerical analysis to build a routine for computing the action of the matrix φ–functions arising in the exponential integration steps, called `bamphi`, able to recycle the information gathered through the exponential integration steps and to reach high levels of speed and accuracy. In this presentation, we outline some of `bamphi`'s main features and ideas.

4 List of participants

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Maierhofer, Georg, 44 R3.07 Z1 Tue 11:15-11:40
Manfredo, Davide, 45 R1.23 Z3 Tue 17:00-17:30
Martin de Diego, David, 45 @ R1.23 Z3 Tue 11:00-11:10
Maslovskaya, Sofya @
Masson, Nicolas @
Mishra, Siddhartha, 46 @ R3.07 Z1 Tue 13:30-14:00
Mitchell, Lawrence, 46 R3.07 Z1 Thu 13:00-13:30
Modin, Klas, 46 @ R3.07, R3.28 @ Z1 Wed 08:10-09:00
Mohammadi, Narges
Moradi, Leila, 47 @ R1.23 Z3 Wed 11:00-11:10
Murari, Davide, 47 R1.23 Z3 Thu 16:30-17:00
Ntarladima, Konstantina
Ober-Blöbaum, Sina, 48 R3.07, R3.28 @ Z1 Thu 10:50-11:40
Offen, Christian, 48 R3.07 Z1 Tue 11:40-12:05
Owren, Brynjulf, 48 R3.07, R3.28 @ Z1 Tue 09:00-09:50
Pagano, Giovanni, 49 @ R1.23 Z3 Wed 10:50-11:00
Palha, Artur, 50 @ R3.07 Z1 Thu 16:30-17:00
Patil, Indrajeet @

Petersson, Andreas, 50 @	R3.28 Z2	Thu 13:30-14:00
Pino Romero, Neisser, 50 @	R1.23 Z3	Tue 11:40-11:50
Plociniczak, Lukasz, 51	R3.28 Z2	Tue 13:30-14:10
Podhaisky, Helmut, 51	R3.28 Z2	Wed 11:30-11:40
Popolizio, Marina, 52	R3.28 Z2	Tue 14:10-14:50
Pulch, Roland, 52	R1.23 Z3	Mon 17:05-17:30
Quispe Mendizábal, Ricardo Angelo @		
Reiter, Philipp, 53	R1.23 Z3	Mon 14:00-14:25
Richter, Thomas, 53 @	R3.07 Z1	Tue 18:00-18:30
Rozza, Gianlugi, 53	R3.07, R3.28 @ Z1	Tue 08:10-09:00
Rufai, Mufutau Ajani, 54 @	R1.23 Z3	Wed 11:30-11:40
Rößler, Andreas, 54 @	R3.28 Z2	Thu 14:00-14:30
Saadat, Mohammad Ali, 54 @	R1.23 Z3	Tue 16:30-17:00
Sato Martín de Almagro, Rodrigo T., 55	R1.23 Z3	Thu 14:30-15:00
Sauter, Henning, 55	R3.28 Z2	Mon 14:50-15:15
Scalone, Carmela, 55 @	R3.28 Z2	Wed 10:50-11:00
Schade, Maximilian, 56	R3.28 Z2	Thu 16:00-16:30
Schratz, Katharina, 56	R3.07, R3.28 @ Z1	Thu 08:10-09:00
Schreiber, Martin, 57 @	R3.07 Z1	Thu 17:00-17:30
Sharma, Akash @		
Shih, Yu-Hsuan, 57 @	R3.07 Z1	Thu 17:30-18:00
Shipton, Jemma, 57	R3.07 Z1	Thu 13:30-14:00
Shourick, Héléna, 58	R3.28 Z2	Mon 15:15-15:40
Skrzypacz, Piotr, 58 @	R3.07 Z1	Wed 11:00-11:10
Stavole, Martina @		
Stern, Ari, 59	R3.07, R3.28 @ Z1	Fri 11:40-12:30
Stillfjord, Tony @		
Strehmel, Karl @		
Tischendorf, Caren, 59	R3.28 Z2	Mon 14:00-14:25
Todesco, Juliano, 60	R1.23 Z3	Tue 14:00-14:30
Tomec, Jan @		
Tromeur-Dervout, Damien, 61	R3.07 Z1	Mon 17:05-17:30
Tumiotto, Denise, 62	R1.23 Z3	Thu 13:00-13:30
Tyranowski, Tomasz, 63	R3.07 Z1	Thu 14:30-15:00
Ul Haq, Ikram @		
Vilmart, Gilles, 63	R3.07, R3.28 @ Z1	Fri 09:00-09:50
Vlaar, Tiffany, 64 @	R3.07 Z1	Tue 17:30-18:00
Voigtmann, Steffen @		
Wang, Han, 65 @	R3.07 Z1	Tue 14:30-15:00
Wang, Mengchao @		
Weinberger, Johanna, 65	R3.28 Z2	Tue 11:15-11:40
Weiner, Rüdiger		
Weiske, Rico, 65	R3.28 Z2	Thu 16:30-17:00
Williamson, Måns, 66 @	R3.28 Z2	Wed 11:20-11:30
Zegeling, Paul Andries, 66	R3.07 Z1	Tue 10:50-11:15
Zhang, Zhen, 66 @	R3.07 Z1	Tue 16:30-17:00
Zimmer, Christoph, 67 @	R3.07 Z1	Wed 11:10-11:20
Zinser, Alexander		
Zivcovich, Franco, 67	R3.07 Z1	Mon 15:15-15:40