Book of Abstracts of NUMDIFF-17

Participants of NUMDIFF-17

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Introduction

This is a draft of the book of abstract of the talks given at NUMDIFF-17, 9–13 September 2024 at the Martin Luther University Halle–Wittenberg. See

`https://sim.mathematik.uni-halle.de/numdiff17`

for more details about the conference.

Fast Multivariate Newton Interpolation for Downward Closed Polynomial Spaces and Applications to Numerical Differential Geometry

Michael Hecht (CASUS - Center for Advanced Systems Understanding Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Görlitz & Mathematical Institute, University Wrocław, Poland), Phil-Alexander Hofmann, Damar Wicaksono, and Michael Hecht

We introduce a fast Newton interpolation algorithm with a runtime complexity of $\mathcal{O}(Nn)$, where N denotes the dimension of the underlying downward closed polynomial space and n its l_p-degree, where $p > 1$. We demonstrate that the algorithm achieves the optimal geometric approximation rate for analytic *Bos-Levenberg-Trefethen functions* in the hypercube. In this case, the Euclidean degree ($p = 2$) emerges as the pivotal choice for mitigating the curse of dimensionality. The spectral differentiation matrices in the Newton basis are sparse, enabling the implementation of fast pseudo-spectral methods on flat spaces, polygonal domains, and regular manifolds.
In particular, we revisit our former contribution, entitled *Global Polynomial Level Sets (GPLS) for Numerical Differential Geometry of Smooth Closed Surfaces*.
The GPLS approximates a broad class of smooth surfaces being only sampled as point clouds by a global polynomial level set, enabling posterior efficient and accurate computation of differential-geometric quantities like mean and Gauss curvature or even 4^{th}-order terms such as the Laplacian of mean curvature. The GPLS significantly reduces the number of surface points required compared to classic alternatives that rely on surface meshes or embedding grids. We sketch extensions to higher dimensions and discuss applications in numerical differential geometry.

HHO Method for Semilinear Sobolev Equation

Ram Jiwari (Indian Institute of Technology Roorkee), Ajeet Singh, N. Kumar

This article presents the development and examination of a hybrid high-order (HHO) approach tailored for solving a semilinear Sobolev equation on polygonal meshes. The HHO method offers distinct advantages over traditional approaches, demonstrating its capability to achieve higher-order accuracy while

reducing the number of unknown coefficients. We establish error approximations for the semi-discrete formulation employing HHO discretization. Using this method we find optimally convergence of orders $\mathcal{O}\left(\tau^2 + h^{k+1}\right)$ in the energy-type norm and $\mathcal{O}\left(\tau^2 + h^{k+2}\right)$ in the L^2 norm.

Two-step Runge-Kutta-Chebyshev methods

Andrew Moisa (Białystok)

Chebyshev (or stabilized) methods are explicit Runge-Kutta methods with extended stability domains along the negative real axis. These methods are intended for large mildly stiff problems, originating mainly from parabolic PDEs.
Two main families of stabilized methods are the most commonly used today:

- Runge-Kutta-Chebyshev methods proposed by van der Houwen & Sommeijer (1980);
- Orthogonal-Runge-Kutta-Chebyshev methods proposed by Abdulle & Medovikov (2001) and Abdulle (2002).

In this talk we consider a new family of two-step Runge-Kutta-Chebyshev methods. It contains

- the second order methods with larger stability intervals than of the one-step methods of this order [1];
- the first-ever third order methods with the closed analytic stability polynomials.

We reveal their theoretical properties, advantages and disadvantages. Also, we discuss the results of numerical experiments and the comparison with widely-known stabilized codes.

References

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Viscoelastic phase separation: Modelling & Structure-preserving discretisation

Aaron Brunk (Johannes-Gutenberg University Mainz, Institute of Mathematics), Aaron Brunk, Maria Lukacova-Medvidova

In the context of binary phase separation dynamic symmetry of both phases, i.e. similar relaxation time scales, plays a crucial role in modelling. The generally accepted model is an incompressible Cahn-Hilliard-Navier-Stokes system for the evolution of the volume fraction and the velocity. In viscoelastic phase separation, this dynamic symmetry is broken, since polymer chains and solvent particles have effects on completely different time scales. To accommodate these asymmetrical effects, the model is extended by additional equations. On one hand, the viscoelastic effects arising from chain dynamics are modeled using the Peterlin model for the conformation tensor. On the other hand, mixing effects between solvent and chains are captured through a nonlinearly coupled advection-reaction-diffusion equation, augmenting the Cahn-Hilliard equation.
In the absence of the conformation tensor, we employ a structure-preserving approximation using conforming finite elements both in space and time. This method is shown to accurately preserve essential thermodynamic quantities, such as conservation of mass and energy dissipation.
Theoretical findings are complemented by a convergence test and an illustrative example drawn from practical applications.

Experiments with a variable-stepsize/variable-order code based on explicit general linear methods

Ali Abdi (University of Tabriz), Zdzislaw Jackiewicz

This talk is about various issues relevant to the development of the code for nonstiff ordinary differential systems based on a class of general linear methods (GLMs) with inherent Runge–Kutta stability (IRKS). These issues include the choice of initial stepsize, computation of the starting vector, construction of continuous interpolants, local error estimation, stepsize and order changing strategies, and updating vectors of external approximations, which propagate from step to step. The resulting experimental code `irks14.m` based on GLMs with IRKS of order $1 \leq p \leq 4$ is tested and compared with

the state-of-art code from the MATLAB ODE suite for the numerical solution of nonstiff ODEs, and it is demonstrated that `irks14.m` is more efficient than `ode45.m` for moderate and stringent tolerances.
Keywords: Ordinary differential equations, General linear methods, Inherent Runge–Kutta stability, Adaptive stepsize and order selection.

Mathematical modeling and simulation of mechano-chemical effect on two-phase avascular tumor

Paramjeet Singh (Thapar Institute of Engineering and Technology), Sweta Sinha

We derive the mathematical model that allows chemotaxis in avascular tumour growth in a two-phase medium. The two phases are the viscous cell phase and the inviscid fluid phase. The conservation of mass-momentum is incorporated in each phase, and appropriate constitutive laws are applied to formulate the governing equations. Further, these equations are simplified into three main variables : cell volume fraction, cell velocity, and nutrient concentration. These variables generate a coupled system of non-linear partial differential equations. A numerical scheme based on the finite volume method is applied to approximate the solution of cell volume fraction. The finite element method is applied to approximate the solutions of cell velocity and nutrient concentration. We investigate tumour growth when when tumour cells move along a fluid containing a diffusible nutrient to which the cells are drawn. We perform some numerical simulations to show the effect of the parameters. The findings of this literature are compatible with the existing literature.

Splitting methods for nonlinear evolution equations

Mechthild Thalhammer (University of Innsbruck, Department of Mathematics)

Exponential operator splitting methods constitute a favourable class of time integration methods for various kinds of linear and nonlinear evolution equations. They rely on the presumption that the defining right-hand side comprises two (or more) operators

$$u'(t) = F\Big(u(t)\Big) = F_1\Big(u(t)\Big) + F_2\Big(u(t)\Big)\,, \quad t \in (0,T)\,,$$

and that the numerical approximation of the associated subproblems

$$u'(t) = F_1\Big(u(t)\Big)\,, \quad u'(t) = F_2\Big(u(t)\Big)\,, \quad t \in (0,T)\,,$$

is significantly simpler compared to the numerical approximation of the original problem. Under these premises, their excellent behaviour with respect to stability, accuracy, and the preservation of conserved quantities has been confirmed by a remarkable amount of contributions.
In my talk, I will review well-known achievements and recent advances on exponential operator splitting methods. As fundamental test problems, I will study Gross–Pitaevskii equations modelling Bose–Einstein condensates, their parabolic counterparts arising in ground and excited state computations, complex Ginzburg–Landau equations having a similar structure, and high-order semilinear parabolic equations describing quasicrystalline patterns. I will contrast standard splitting schemes involving real coefficients with two alternative approaches that are based on the incorporation of complex coefficients or double commutators, respectively. Besides, I will sketch the formal calculus of Lie derivatives, which provides powerful tools regarding the design and analysis of splitting methods in the context of nonlinear evolution equations.

Resolving singularities in parabolic initial-boundary value problems

Torsten Linß (FernUniversität in Hagen), Brice Girol

We consider a time-dependent reaction-diffusion equation with a singularity arising from incompatible initial and boundary conditions:

$$u_t - u_{xx} + b(x,t)u = f \qquad \text{in } \ (0,\ell) \times (0,T],$$

subject to boundary conditions

$$u(0,t) = \varphi_0(t), \quad u(\ell,t) = \varphi_\ell(t), \quad t \in (0,T],$$

and the initial condition

$$u(x,0) = 0, \qquad x \in (0,\ell)\,,$$

with $\varphi_0(0) \neq 0$.
The discrepancy between initial and boundary conditions causes the formation of a singularity in the vicinity of the corner $(0,0)$. This singularity s can be characterised as the solution of

$$s_t - s_{xx} + b(0,0)s = 0 \qquad \text{in} \quad (0,\infty) \times (0,T],$$

subject to the boundary condition

$$s(0,t) = \varphi_0(0), \quad t \in (0,T],$$

and the initial condition

$$s(x,0) = 0, \qquad x \in (0,\infty)\,.$$

This in turn can be given analytically using the error function. Then the interesting question is:

How can the remainder $y = u - s$ be resolved numerically?

We derive bounds on the derivatives of the remainder y — under significantly less restrictive assumptions then previously assumed by other authors — and show how a numerical approximation can be obtained using an appropriately designed mesh.

First-kind Galerkin BEM for the Hodge-Helmholtz equation

Anouk Wisse (TU Delft), Ralf Hiptmair, Carolina Urzúa-Torres

We are interested in exterior boundary value problems (BVP) for the Euclidean Hodge-Helmholtz operator $-\Delta_{HH} := \mathbf{curl}\,\mathbf{curl} - \eta\nabla\mathrm{div} - \kappa^2$, which is closely related to Maxwell equations in frequency domain. In order to solve these exterior BVPs, we consider the corresponding first-kind boundary integral equations, which were derived and analyzed in [2]. It is worth noticing that the boundary integral operators (BIOs) for Hodge-Helmholtz induce bounded and coercive sesquilinear forms in their natural energy trace spaces, and one can establish the unique solvability of the related first-kind boundary integral equations. However, the situation changes when the wavenumber κ is zero, i.e., for the Hodge-Laplacian. Then, the related BIOs feature kernels whose dimensions are linked to fundamental topological invariants of the domain Ω. Moreover, Galerkin discretization does not affect the dimensions of these kernels [3].

In this talk, we pursue the Galerkin discretization of the variational formulations in [2] and we provide numerical experiments for these boundary integral equations using Bempp [1]. We validate our implementation using a new Calderón residual technique. Then, we compare the eigenvalues related to the equivalent saddle point formulation for $\kappa = 0$ with those found in [3] and also present the spectra for small wave numbers κ and discuss its numerical consequences.

References

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Analysis of stochastic viral infection models with budding and bursting strategies

Sonjoy Pan (VIT Bhopal University)

Stochastic viral infection models with two modes of infection transmission (virus-to-cell and cell-to-cell) as well as antibody response, are presented. The budding and bursting strategies for the release of virions are taken into consideration in the formulation of the stochastic differential equation models. The stochastic means and standard deviations of the uninfected and infected cells, viruses, and antibodies are numerically computed and graphically compared with the results obtained from the deterministic models. The results demonstrate that the likelihood of viruses going extinct is dependent not only on whether the basic reproduction number is greater than unity but also on the initial viral load. The numerical findings also imply that, in the case of budding as compared to bursting strategy, the probability of virus extinction is relatively higher.

Half-Explicit Runge-Kutta Lie Group Integrators for Flexible Multibody Systems

Denise Tumiotto (Martin Luther University Halle-Wittenberg, Institute of Mathematics), Martin Arnold

When modelling geometrically exact beams under constraints, two problems arise: The presence of nonlinear configuration spaces for describing large rotations and the presence of algebraic variables coupled with differential ones. To obtain an efficient numerical solution for the latter problem, half-explicit Runge-Kutta methods have been introduced in 1992 by Brasey and Hairer. The current work adapts these half-explicit Runge-Kutta methods to solve index-2 DAEs in nonlinear configuration spaces, of the Lie group form, so that the first problem is covered. Nevertheless, a well-known issue, called drift-off effect, rises when evaluating the numerical solution of reduced index DAEs. Specifically, when reducing the index from 3 to 2 by differentiation of the constraints, we introduce new constraints at velocity level and numerical residuals in the constraints at position level. Previous techniques of projection or stabilization to avoid the drift-off effect are adapted to the case of interest. To conclude the study, numerical experiments on flexible structures modelled as Cosserat rods are performed.

Schwarz Time Domain Decomposition with spectral Tchebychev time integration

Damien Tromeur-Dervout (Université Claude Bernard Lyon 1, Institut Camille Jordan UMR5208 CNRS-UCBL)

This talk focuses on a Schwarz time domain decomposition applied to system of nonlinear ordinary differential equations (ODEs) for initial values problem (IVP) based on the transformation of the original IVP into a boundary values problem (BVP). The method consists of splitting the time interval in time slices and integrating the BVP on each time slice with nonlinear transmission conditions associated with the conservative form of the BVP between the time slices. However, constraints on the size of the time slices appear in the resolution of the BVP. We investigate the use of spectral implicit time integration using a Gauss-Lobatto distribution of time steps over each time slice that allows an implicit adaptation of the size of the time slices involved

in the time decomposition. Results obtained on the Lotka-Volterra prey-predator problem will be presented.

Wavelets based physics informed neural networks to solve non-linear differential equations

Ziya Uddin (BML Munjal University), Sai Ganga

This work presents the numerical solution of Blasius boundary layer fluid flow 2-dimensional fluid flow problem using unsupervised physics-informed neural networks. The applicability of different wavelets as activation functions is investigated. As PINN depends on various parameters, the impact of network architecture on the accuracy of the model is also studied. The findings show that wavelet activation functions can offer improved accuracy over the traditional tanh activation function, depending on the specific problem, demonstrating the potential for enhanced performance with the proposed method.

Peer methods for the numerical solution of general second order IVPs

Luis Randez (University of Zaragoza), Manuel Calvo, Juan Ignacio Montijano

In this work, we solve numerically general second order initial vale problems $y'' = f(t, y, y')$ by means of explicit two-step Peer methods, given by

$$\begin{aligned} Y_{m+1} &= BY_m + hAZ_m + h^2QF_{m-1} + h^2RF_m, \\ Z_{m+1} &= \widehat{B}Z_m + h\widehat{Q}F_{m-1} + h\widehat{R}F_m, \end{aligned} \tag{1}$$

where the stage vectors evaluated at $t_{mi} = t_m + c_i h$ are

$$\begin{aligned} Y_m &= (Y_{mi}), \text{ where } Y_{mi} \simeq y(t_{mi}), \\ Z_m &= (Z_{mi}), \text{ where } Z_{mi} \simeq y'(t_{mi}), \\ F_m &= (f(t_{mi}, Y_{mi}, Z_{mi})). \end{aligned} \tag{2}$$

We propose explicit Peer methods with minimum number of effective function evaluations per step. We analyze the 0-stability, consistency and convergence of these schemes.

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Generating non-stationary Gaussian random fields on hypersurfaces using surface finite element methods

Erik Jansson (Chalmers University of Technology and University of Gothenburg), Annika Lang, Mike Pereira

In the middle of the previous century, Peter Whittle demonstrated that Whittle–Matérn Gaussian random fields on Euclidean domains can be obtained as solutions to fractional elliptic stochastic partial differential equations (SPDEs). The SPDE–random field connection can be leveraged to generate random fields on other domains, such as curves or surfaces, by solving an SPDE on that domain. Selecting a differential operator with variable coefficients, we obtain a flexible class of non-stationary random fields. We consider how the computational technique of surface finite elements can be utilized to generate random fields on surfaces and briefly discuss how strong error bounds are obtained using complex analysis and operator theory. This talk is based on joint work with Annika Lang and Mike Pereira.

Computing the matrix exponential and the Cholesky factor of a related finite horizon Gramian

Tony Stillfjord (Lund University, Centre for Mathematical Sciences), Filip Tronarp

The solution to a differential Lyapunov equation can be expressed in closed form as a matrix-valued integral, the so-called finite-horizon Gramian. Such Gramians also have applications in many other areas, such as Gauss-Markov regression. The Gramian is positive semi-definite, and often it is more useful to have a Cholesky factorization of it rather than the Gramian itself. I will present a new efficient numerical method for computing such Cholesky

factors of finite-horizon Gramians without first computing the full Gramian. In contrast to other methods applicable to this task, this method is a generalization of the scaling-and-squaring approach for approximating the matrix exponential. It exploits a similar doubling formula for the Gramian, and thereby keeps the required computational effort modest. Most importantly, we have performed a rigorous backward error analysis that guarantees that the approximation is accurate to the round-off error level in double precision if the method parameters are chosen appropriately. I will sketch the outline of this proof. I will also show the results of supporting numerical experiments on a large number of standard test cases, which illustrate that this accuracy is indeed achieved in practice.

Waveform iteration for ocean-atmosphere-sea-ice coupling

Philipp Birken (Lund University), Valentina Schüller, Eric Blayo, Florian Lemarié

Within Earth system models (ESM), many differential and algebraic equations are coupled together. Thereby, different submodels are implemented in separate codes that use their own discretization and time step, a so called partitioned approach. Here, we consider the coupling between ocean, atmosphere and sea ice. The first two models are based on PDEs on separate but connected domains, and exchange information via boundary conditions. The sea ice model is a lower dimensional PDE, coupled to the ocean solver.
Our general aim is to understand the coupling error caused by this approach, and to suggest improvements. To this end, we treat this as part of a waveform relaxation method. These consider two coupled ODEs and solve them iteratively, given data from the respective other equation. Note that in ESM, only one iteration is performed.
We implemented a true waveform relaxation method in the single column version of the European ESM EC-Earth [1]. This way, we can get a reference solution per time window, and thus observe the coupling error. We see that there is a small but clearly noticable coupling error for pure ocean-atmosphere coupling, and that the inclusion of sea-ice makes this worse.

References

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Autoencoders for structure-preserving model reduction of stochastic Hamiltonian systems

Tomasz Tyranowski (University of Twente, Department of Applied Mathematics), Benedikt Brantner

As recently shown (Tyranowski, 2024), SVD-based model reduction techniques, such as the proper orthogonal decomposition, can be extended to stochastic differential equations in order to reduce the computational cost arising from both the high dimension of the system and the large number of independent Monte Carlo runs. These techniques offer a significant computational efficiency improvement when the Kolmogorov n-width of the solution manifold of the considered problem decays quickly with the dimension of the reduced space. In this work, we adapt the recently proposed symplectic autoencoders (Brantner & Kraus, 2023; Buchfink, Glas & Haasdonk, 2023) to the stochastic setting and apply them to stochastic Hamiltonian systems characterized by slowly decaying Kolmogorov n-widths. The performance of thus constructed model reduction methods is tested and compared to the linear proper symplectic decomposition method.

Convergence analysis of a finite volume scheme for a stochastic Allen-Cahn problem

Aleksandra Zimmermann (Institute of Mathematics TU Clausthal), Caroline Bauzet, Cedric Sultan, Guy Vallet

We address the convergence analysis of a numerical scheme for an Allen-Cahn problem with constraint and with a stochastic external force given by a multiplicative noise of Itô type. The problem is set up in a bounded spatial domain of dimension 2 or 3 and homogeneous Neumann boundary conditions are considered.
We propose a time-space discretization, of semi-implicit Euler-Maruyama type with respect to time and a Two-Point Flux Approximation (TPFA) with respect to space for a regularized version of the constrained problem. Under the assumption $\Delta t = \mathcal{O}(\epsilon^{2+\theta})$ for a positive θ on the time parameter Δt and the regularization parameter ϵ we show the convergence our scheme towards the unique variational solution of the problem.

Two Discretisations of the Time-Dependent Bingham Problem

Mira Schedensack (Universitaet Leipzig, Mathematisches Institut), Carsten Carstensen

This talk introduces a non-conforming Crouzeix-Raviart approximation of the stationary three-dimensional Bingham problem and the two-dimensional Mosolov problem for the flow in a pipe. The non-conformity allows for quasi optimal error estimates in contrast to the standard conforming $P1$ finite element scheme. Moreover, this space discretisation is combined with two time-discretisations for the corresponding time-dependent problems. The first time discretisation is a generalised midpoint rule and the second time discretisation is a discontinuous Galerkin scheme. The a priori error analyses for both schemes yield certain convergence rates in time and optimal convergence rates in space. It guarantees convergence of the fully-discrete scheme with a discontinuous Galerkin time-discretisation for consistent initial conditions and a source term $f \in H^1(0,T;L^2(\Omega))$.

Implicit Peer Triplets in ODE Constrained Optimal Control

Jens Lang (Technische Universität Darmstadt), Bernhard A. Schmitt

Recently, we have developed and analyzed implicit two-step Peer triplets for nonlinear ODE constrained optimal control problems [Journal of Computational and Applied Mathematics 416:114596, 2022, Algorithms 15:310, 2022]. We combine some standard Peer methods for inner grid points with carefully designed starting and end methods to achieve order four for the state variables and order three for the adjoint variables in a first-discretize-then-optimize approach. The notion triplets emphasizes that these three different Peer methods have to satisfy additional matching conditions. These methods do not suffer from order reduction – a phenomenon that is usually observed for one-step methods as e.g. symplectic Runge-Kutta methods. Peer methods compute several stages of equal (global) order per time step. They exhibit good stability properties, making them very attractive for stiff problems [Applied Numerical Mathematics 53:457-470, 2005]. In this talk, we will present novel implicit two-step Peer triplets, which can be applied together with a projected gradient method [`https://arxiv.org/abs/2303.18180v2`]. The key observation is that such methods have to satisfy further positivity and

consistency conditions. We will also discuss the use of variable stepsizes together with the property of super-convergence [https://arxiv.org/abs/2404.13716]. Several numerical examples will be presented.

On PDE convergence of AMF-TASE W-methods for multidimensional linear parabolic problems

Domingo Hernández Abreu (Universidad de La Laguna), S. González Pinto, G. Rivero Herrera

This talk deals with the time-integration of space-discretised parabolic problems subject to Dirichlet boundary conditions on a rectangular m-dimensional domain. We consider a class of linearly implicit methods (TASE W-methods, [2]) in combination with Approximate Matrix Factorization [1] based on an alternating direction implicit approach, which allows to reduce the algebra cost to the level of one-dimensional problems. Optimal results on PDE-convergence will be presented for linear problems, the Euclidean norm and arbitrary spatial dimensions $m \geq 2$. Numerical experiments will be presented to assess the PDE-convergence results.

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Convergence analysis of Lie and Strang splitting applied to operator-valued differential Riccati equations

Teodor Åberg (Lund University, Centre for Mathematical Sciences), Tony Stillfjord

Differential Riccati equations (DREs) are matrix-valued or operator-valued equations with quadratic nonlinearities that arise in many areas. Most importantly, in control theory, where their solutions provide the optimal feedback control laws for linear quadratic regulators on finite time intervals. There are numerous numerical methods for DREs, but most of these lack proper (temporal) convergence analyses. The few existing analyses consider the matrix-valued case, and rely on properties that may not necessarily hold in the operator case. This is problematic when the matrix-valued DRE arises from a spatially discretized operator-valued DRE, corresponding to the control of a partial differential equation. In this case, refining the spatial discretization increases the problem dimension, and might cause the temporal errors to grow uncontrollably.
In view of this, we provide rigorous convergence analyses of two numerical time-stepping methods, the Lie and Strang splitting schemes, when applied to operator-valued DREs. We show that they achieve the standard orders of convergence under different types of (low) regularity assumptions. Essentially, either the initial condition or the operator giving rise to the nonlinearity should be smoothing to a certain degree, but not necessarily both. We illustrate these theoretical results with several numerical experiments on DREs arising from the control of partial differential equations.

A Lie group generalized-α method with improved accuracy

Martin Arnold (Martin Luther University Halle-Wittenberg), Johannes Gerstmayr, Stefan Holzinger

Lie group integrators solve initial value problems for (ordinary) differential equations on manifolds with Lie group structure. For one-step methods, the application of classical ODE time integration methods to a locally defined equivalent ODE in terms of local coordinates has become a quasi-standard. These local coordinates are elements of the corresponding Lie algebra. They are mapped by the exponential map or by the Cayley map to the Lie group itself. For typical fields of application, there are closed form expressions that allow to evaluate these coordinate maps and the right hand side of the locally defined equivalent ODE efficiently.
For multi-step methods and for the generalized-α method with its subsidiary variables, the situation is more complex since frequent re-parametrizations of

the manifold need to be avoided. As a practical consequence, the corresponding Lie group methods suffer from extra local error terms that may, however, be eliminated by appropriate correction terms (V. Wieloch, M. Arnold: *BDF integrators for mechanical systems on Lie groups*, NUMDIFF-15, 2018). Recently, these modified Lie group integrators have been interpreted in terms of time derivatives of the local coordinates. In that way, the accuracy of simulation results was substantially improved (S. Holzinger, M. Arnold, J. Gerstmayr: *Improving the accuracy of Newmark-based time integration methods*, IMSD 2024, June 2024).
In the present paper, we analyse local and global errors of these modified generalized-α methods, discuss some implementation issues and present numerical test results that illustrate the improved accuracy.

Intrinsic Projection (IP) of Implicit Runge Kutta Methods for Differential Algebraic Equations

Nikita Kapur (University of Iowa, USA.), Laurent Jay

We present the new technique of Intrinsic Projection (IP) for Implicit Runge-Kutta (IRK) Methods applied to differential-algebraic equations (DAEs). IP does not require the accurate evaluation of any additional Jacobian like for standard Projected Implicit Runge-Kutta Methods and is therefore simpler to implement. IP for IRK methods is analyzed for index 2 DAEs, in particular we give results about existence and uniqueness, and some error estimates. For index 2 DAEs IP for IRK methods is shown to lead to the same order of error estimates as standard Projected Implicit Runge-Kutta Methods, but at a lower computational cost. Some preliminary results for index 3 DAEs will also be given.

Convergence rates for a finite volume scheme of the stochastic heat equation

Niklas Sapountzoglou (Clausthal University of Technology, Institute of Mathematics), Aleksandra Zimmermann

In this contribution, we provide convergence rates for a finite volume scheme of the stochastic heat equation with multiplicative Lipschitz noise and homogeneous Neumann boundary conditions (SHE). More precisely, we give an

error estimate for the L^2-norm of the space-time discretization of SHE by a semi-implicit Euler scheme with respect to time and a TPFA scheme with respect to space and the variational solution of SHE. The only regularity assumptions additionally needed is spatial regularity of the initial datum and smoothness of the diffusive term.

Hessian-free force-gradient integrators

Kevin Schäfers (University of Wuppertal), Jacob Finkenrath, Michael Günther, Francesco Knechtli

This talk deals with the framework of Hessian-free force-gradient integrators [1] for separable Hamiltonian systems of the form

$$H(p,q) = \frac{1}{2}p^\top M p + V(q).$$

Unlike traditional force-gradient integrators [2], the Hessian-free variants do not require the analytical expression of the force-gradient term, which includes the Hessian of the potential. Instead, the force-gradient update is approximated, effectively replacing the force-gradient term with an additional force evaluation. We examine the order conditions and discuss the geometric properties of the proposed numerical integration schemes. Moreover, we perform a linear stability analysis of (Hessian-free) force-gradient integrators and identify promising self-adjoint methods. Numerical experiments will be presented, highlighting the advantages and disadvantages of the Hessian-free variants.

References

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Probabilistic Time Integration for Semi-explicit PDAEs

Afsaneh Moradi (Otto-von-Guericke Universität Magdeburg), Robert Altmann

This talk is about the application of probabilistic time integration methods to semi-explicit partial differential–algebraic equations of parabolic type and its semi-discrete counterparts, namely semi-explicit differential–algebraic equations of index 2. The proposed methods iteratively construct a probability distribution over the solution of deterministic problems, enhancing the information obtained from the numerical simulation. The efficacy of the randomized versions of the implicit Euler method, the midpoint scheme, and exponential integrators of first and second order are examined. By demonstrating the consistency and convergence properties of these solvers, their utility in capturing the sensitivity of the solution to numerical errors is illustrated. Our analysis establishes the theoretical validity of randomized time integration for constrained systems and offers insights into the calibration of probabilistic integrators for practical applications.

Stabilization of a matrix via a low-rank-adaptive ODE

Stefano Sicilia (Gran Sasso Science Institute), Nicola Guglielmi

Let A be a square matrix with a given structure (e.g. real matrix, sparsity pattern, Toeplitz structure, etc.) and assume that it is unstable, i.e. at least one of its eigenvalues lies in the complex right half-plane. The problem of stabilizing A consists in the computation of a matrix B, whose eigenvalues have all negative real part and such that the perturbation $\Delta = B - A$ has minimal norm. The structured stabilization further requires that the perturbation preserves the structural pattern of A. This non-convex problem is solved by a two-level procedure which involves the computation of the stationary points of a matrix ODE. It is possible to exploit the underlying low-rank features of the problem by using an adaptive-rank integrator that follows rigidly the rank of the solution. Some benefits derived from the low-rank setting are shown in several numerical examples. These computational advantages also allow to deal with high dimensional problems.

Efficient Numerical Methods for Fractional Differential Equations

Afshin Farhadi (Technical University of Applied Sciences Würzburg-Schweinfurt, Faculty of Applied Natural Sciences and Humanities (FANG))

The approximate evaluation of fractional Riemann-Liouville integrals in their traditional representation leads to complex computations that require a relatively high memory and large amount of time when they are implemented on a computer. In this talk, our aim is to introduce the concept of a so-called diffusive representation (or infinite state representations). This is an approach on which we can construct very efficient numerical algorithms with respect to both the run time and the memory issues for computing fractional integrals. Indeed such representations can lead to numerical methods with small run time and low memory requirements. We additionally show how one can apply such diffusive-representation-based algorithms to solve fractional ordinary differential equations in a fast and highly accurate way.

The work presented in this conference is related to a joint project with Prof. Kai Diethelm and Dr. Renu Chaudhary (THWS) and Dr. André Schmidt and Paul E. Haacker (Institute of Nonlinear Mechanics, Universität Stuttgart). This project is supported by the German Federal Ministry of Education and Research (BMBF) under Grant 05M22WHA.

A quasi-optimal space-time finite element method for parabolic equations

Rob Stevenson (University of Amsterdam, Korteweg-de Vries Institute for Mathematics), Lars Diening, Johannes Storn

We outline the (potential) advantages of simultaneous space-time discretisations of parabolic evolution equations, and illustrate them with some numerical results.
Other than with elliptic equations there is not one obvious variational formulation, and we present several possibilities. They have in common that the bilinear form is not coercive so that one has to resort to minimal residual

discretisations, in most cases in a dual norm which leads to a saddle point problem.
For one specific choice of a variational formulation, we present some technical details concerning adaptive mesh refinement, the construction of uniformly bounded Fortin interpolators, and optimal preconditioning.

A fully discretized domain decomposition approach for semi-linear SPDEs

Marvin Jans (Lund University), Monika Eisenmann, Eskil Hansen

We consider a fully discretized numerical scheme for parabolic stochastic partial differential equations with additive or multiplicative noise. Our method is based on a non-iterative domain decomposition approach. Such methods can help parallelize the code and therefore lead to a more efficient implementation.

The domain decomposition is integrated through an operator splitting approach, where one operator acts on one part of the domain. More precisely, we combine the implicit Euler method with the Douglas-Rachford splitting scheme. For an efficient space discretization of the underlying equation, we chose the discontinuous Galerkin method. For this fully discretized scheme, we provide a strong space-time convergence result.

In the presentation, the numerical method will be explained, together with a short outline of the convergence proof. We conclude the presentation with numerical experiments validating our results.

A matrix-oriented approach for the numerical solution of a metal corrosion model

Gianluca Frasca-Caccia (University of Salerno, Department of Mathematics), Dajana Conte, Beatrice Paternoster

One of the main challenges in the numerical solution of corrosion models is the development of efficient numerical methods that can be used for predictive maintenance.

In this talk we consider a phase field model for metal pitting corrosion that allows for a simple and autonomous treatment of the moving interface. However, the equation that models the front evolution is highly stiff. The use of explicit time integrators after a standard space discretization is unpractical, due to strict stability requirements that force the use of tiny time steps.
Based on the Kronecker-sum structure of the discrete Laplacian obtained from standard finite difference approximations, we propose an efficient implementation of IMplicit-EXplicit (IMEX) time integrators.
Numerical tests are proposed to compare the proposed techniques with others from the literature.

A posteriori error bounds for pseudo parabolic problems using C_0 semigroups

Martin Ossadnik (FernUniversität in Hagen), Torsten Linß

We consider the second-order pseudo parabolic equation of finding $u : [0, T] \mapsto H_0^1(\Omega)$, $\Omega \subset \mathbb{R}^d$, such that

$$\mathcal{L}\partial_t u(t) + \mathcal{M}u(t) = F(t) \quad \text{in } (0, T] \tag{3}$$

with two second order, elliptic operators $\mathcal{L}, \mathcal{M} : H_0^1(\Omega) \mapsto H^{-1}(\Omega)$ and a source function $F : [0, T] \mapsto H^{-1}(\Omega)$. Furthermore an initial condition

$$u(0) = u_0, \quad u_0 \in H_0^1(\Omega), \tag{4}$$

is given. We will assume, that the operator $\mathcal{M}$ is bounded and that $\mathcal{L}$ is both bounded and coercive.
A computable a posteriori error bound in a weighted H^1-norm for a full discretisation using the backward differential formula of order two (BDF-2 method) in time and $\mathbb{P}_2$-elements in space is derived. To do so, we leverage the C_0 semigroup, generated by the operator $\mathcal{L}^{-1}\mathcal{M}$. Furthermore we adapt elliptic reconstructions introduced by C. Makridakis and R. N. Nochetto to pseudo parabolic problems.

Given some numerical results we analyze the estimate's order, efficiency and components. Last but not least, we show that we can apply our a posteriori error bound to other time discretisations like the backward Euler and Crank Nicolson method.

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The algebraic and geometric structures of exotic aromatic Butcher series for the backward error analysis of ergodic stochastic differential equations

Adrien Laurent (Inria Rennes), Eugen Bronasco, Hans Munthe-Kaas

The exotic aromatic Butcher series formalism is a strong tool for the creation of high-order integrators for sampling the invariant measure of ergodic SDEs. In this talk, we uncover a universal geometric characterisation of exotic aromatic series and the Hopf algebra structures related to the composition and substitution laws of exotic aromatic series. In particular, we describe backward error analysis with exotic aromatic series and give an explicit expression of the modified vector field at any order.

Legendre wavelet collocation method for stochastic fractional integro-differential equation

Abhishek Kumar Singh (University of Greifswald), Mani Mehra

The numerical methods based on operational matrices for the fractional differential equations have been widely studied in the last decade. In the wavelet method based on orthogonal polynomials, the operational matrices for wavelets are derived using other functions (block pulse and hat function) that lead to an approximation error. In contrast to the existing methods, here we derive the expressions for operational matrices without using the usual block pulse and hat function, aiming to remove the approximation error. Furthermore, we design a Legendre wavelet collocation method involving different operational matrices for solving the stochastic fractional integro differential equation (SFIDE). Thereafter, making use of the wavelet approximation, operational matrices, and collocation points, we convert the considered SFIDE into a system of algebraic equations. Finally, we investigate the accuracy and efficiency of the numerical method through test examples.

Stochastic backward error analysis: application to Hamiltonian systems

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

In this talk, we address our attention on the geometric numerical integration of stochastic Hamiltonian systems, under the backward error analysis perspective. Firstly, we consider symplectic numerical integrators for canonical stochastic Hamiltonian systems. In order to gain insights on the behaviour of the long-term Hamiltonian error that arises along the aforementioned numerical dynamics, we construct stochastic modified equations, whose exact solutions coincide with such numerical ones. Then, a rigorous study of such exact solutions will follow to capture the eventual conservative properties of the associated numerical methods. This methodology will allows us to get an extension of the well-known *Benettin-Giorgilli Theorem* to the stochastic scenario, explaining the long-term trend of Hamiltonian errors along symplectic numerical integrators. Then, the extension to the case of stochastic Poisson systems will be also studied. In this scenario, the aim is to detect the behaviour of stochastic Poisson integrators, in terms of preserving the Hamiltonian function associated to the so-called *Wong-Zakay approximating system*, i.e., a stochastic system obtained upon approximating the Wiener process with a linear (in time) combination of Wiener increments. Finally, a selection of numerical experiments will be displayed, confirming the effectiveness of the theoretical analysis. This is a joint project with Raffaele D'Ambrosio (University of L'Aquila).

A class of composite barycentric rational Hermite quadrature method for Volterra integral equations

Seyyed Ahmad Hosseini (Golestan University), Ali Abdi, Kai Hormann

Barycentric rational interpolation offers an elegant approach to avoid a common problem of rational interpolation, namely the occurrence of poles in the interpolation interval, which is undesirable in many situations. More recently, Cirillo and Hormann [1] introduced an iterative approach to the Hermite rational interpolation problem. The main theme of this talk is to introduced quadrature rules based on barycentric rational Hermite interpolation. To this end, a barycentric rational Hermite quadrature, and a composite version of

that will be introduced. Then, the proposed composite quadrature formula will be utilized to construct a direct method for solving Volterra integral equations (VIEs)

$$y(t) = g(t) + \int_{t_0}^{t} k(t, s, y(s))\,\mathrm{d}s, \qquad t \in I = [t_0, T], \tag{5}$$

where $g\colon I \to \mathbb{R}^D$ and $k\colon S \times \mathbb{R}^D \to \mathbb{R}^D$ are given functions, D stands for the dimension of the system, and $S = \{(t, s) : t_0 \le s \le t \le T\}$. To show the efficiency of the proposed method in solving VIEs and to validate the theoretical results, some numerical verifications will be presented.
Keywords: Linear barycentric rational interpolation, Hermite interpolation, Quadrature, Volterra integral equations.

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Prediction of information diffusion through epidemiological models

Samira Iscaro (University of Salerno), Dajana Conte, Beatrice Paternoster

Information diffusion on social media is a quite complex phenomenon to be analyzed, since these are free and easily accessible to anyone who has an Internet connection and a proper device. There are several mathematical approaches to carry out this kind of analysis: one of these consists of using epidemiological models based on ordinary differential equations [2, 3, 4]. However, describing only the evolution of the phenomenon is not sufficient, but it is even required to predict its evolution.
The main aim of this talk is to highlight how, using a proper parameter estimation strategy and an adequate dataset, built using real data, it is possible to obtain the desired predictions [1], as showed by numerical tests realized studying real news spread on the social network X (Twitter) during the period 2020-2022.

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Finite element approximation of the Monge-Ampère equation

Dietmar Gallistl (University Jena), Ngoc Tien Tran (Universität Augsburg)

The Monge–Ampère equation

$$\det D^2 u = f \text{ in } \Omega \quad \text{and} \quad u = g \text{ on } \partial\Omega$$

in a convex domain Ω with suitable data f, g admits a unique generalized solution in the cone of convex functions. The use of high-order methods or local mesh refinement is very desirable for the discretization of the above problem. On the other hand, a stable algorithmic realization of the finite element method is difficult to achieve due to the strong nonlinearity and the convexity constraint.
This talk discusses a regularization approach through uniformly elliptic Hamilton–Jacobi–Bellman equations. The regularized problem possesses a unique strong solution u_ε and is accessible to the discretization with finite elements. The contribution establishes locally uniform convergence of u_ε to the convex Alexandrov solution u to the Monge–Ampère equation as the regularization parameter ε approaches 0. A finite element method for the approximation

of u_ε is proposed, and the regularized finite element scheme is shown to be locally uniformly convergent. Based on Alexandrov's estimate, some a posteriori error estimates are also shown.

Stable and positivity preserving solvers for time-fractional reaction-advection-diffusion problems

Angelamaria Cardone (University of Salerno), Gianluca Frasca Caccia, Beatrice Paternoster

Reaction-advection-diffusion problems, where the memory effect plays an important role, may be successfully modeled by partial differential equations with a fractional derivative in time. In the numerical simulation, main concerns regard the accuracy, since most standard schemes exhibit low order of convergence; the computational cost, due to the discretization of the history term. Moreover, in real applications, another issue is the preservation of qualitative properties of the analytical solution, which is usually achieved only for small stepsizes. Here, we propose two pairs of nonstandard time-stepping methods, which are unconditionally stable and positivity preserving. The analysis of these methods is illustrated and some numerical experiments are shown for comparison with classical methods.

Regularity and numerical approximation of fractional elliptic differential equations on compact metric graphs

Mihály Kovács (Pázmány Péter Catholic University), David Bolin, Vivek Kumar, Alexandre B. Simas

The fractional differential equation $L^\beta u = f$ posed on a compact metric graph is considered, where $\beta > 0$ and $L = \kappa^2 - \nabla(a\nabla)$ is a second-order elliptic operator equipped with certain vertex conditions and sufficiently smooth and positive coefficients κ, a. We demonstrate the existence of a unique solution for a general class of vertex conditions and derive the regularity of the solution in the specific case of Kirchhoff vertex conditions. These results are extended to the stochastic setting when f is replaced by Gaussian white noise. For the deterministic and stochastic settings under generalized Kirchhoff vertex conditions, we propose a numerical solution based on a

finite element approximation combined with a rational approximation of the fractional power $L^{-\beta}$. For the resulting approximation, the strong error is analyzed in the deterministic case, and the strong mean squared error as well as the $L_2(\Gamma \times \Gamma)$-error of the covariance function of the solution are analyzed in the stochastic setting. Explicit rates of convergences are derived for all cases. Numerical experiments for $L = \kappa^2 - \Delta, \kappa > 0$ are performed to illustrate the results.

New efficient linearly implicit numerical methods for stiff huge differential problems

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

Partial Differential Equations (PDEs) are used for modeling various phenomena. We are interested in the efficient numerical solution of PDEs from applications, such as: a DIB (Dual-Ion Batteries) model for the formation of spatio-temporal patterns in electrodeposition in batteries [3]; models for the evolution of vegetation in environments characterized by specific conditions such as soil aridity, rainfall periodicity, and so on [5]. The spatial discretization of these models leads to huge stiff initial value problems. In this talk, we derive a new class of linearly implicit numerical methods capable of solving the mentioned problems accurately, employing reasonable computing times, and reproducing the expected Turing patterns.
The proposed methods constitute a generalization of the TASE-RK (Time-Accurate and highly-Stable Explicit Runge-Kutta) numerical schemes introduced by Bassenne et al. and Calvo et al. in 2021 [2, 4]. The latter make use of appropriate preconditioners, called TASE operators, to improve the stability of explicit RK methods. The new methods, called GTRK (Generalized TASE-RK) [1], are derived using different TASE operators for each stage of the underlying explicit RK scheme. By exploiting connections between GTRK methods and W-methods for the study of consistency, we show that it is possible to drastically reduce the number of linear systems required by classical TASE-RK schemes to reach order $p \leq 4$. Furthermore, we construct A-stable GTRK methods of order $p = 2, 3, 4$. The numerical experiments show the better efficiency of the proposed methods over the classical TASE-RK schemes, and over other linearly implicit numerical methods from the scientific literature.

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Computing the stationary measure of McKean-Vlasov SDEs

Jean-François Chassagneux (Université Paris Cité, LPSM), Gilles Pagès (Sorbonne Université)

Under some confluence assumption, it is known that the stationary distribution of a McKean-Vlasov SDE is the limit of the empirical measure of its associated self-interacting diffusion. Our numerical method consists in introducing the Euler scheme with decreasing step size of this self-interacting diffusion and seeing its empirical measure as the approximation of the stationary distribution of the original McKean-Vlasov SDEs. This simple approach is successful (under some raisonnable assumptions...) as we are able to prove convergence with a rate for the Wasserstein distance between the two measures both in the L2 and almost sure sense. In this talk, I will first explain the rationale behind this approach and then I will discuss the various convergence results we have obtained.

Cell seeding dynamics in a porous scaffold material with applied sensitivity analysis

Henry Jäger (Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Department of Mathematics), Bernd Simeon

In this presentation, we report about ongoing work on in silico research for the better understanding of an experimental study for meniscus regeneration. In essence, this experiment uses a nonwoven scaffold that is colonized by human mesenchymal stem cells and chondrocytes. The mathematical description involves active processes at the cell level, such as cell differentiation and matrix synthesis, that have a strong impact on the resulting tissue structure and quality, while macroscopic effects in turn are important stimuli for the processes at the microscopic level. The corresponding mathematical model consists of a set of coupled nonlinear parabolic partial differential equations where further effects, such as the flow of nutrients through the porous media of the scaffold and the mechanical deformation, can also be taken into account. From the numerical point of view, not only the forward simulation with vastly differing time scales but also the computation of parameter sensitivities represents a big challenge. Besides presenting the results of current simulations of the experiment, the talk concentrates on investigating different approaches for calculating sensitivities. In particular, a classical approach where sensitivities are directly computed is compared to a statistical approach using Sobol' indices. This new approach also utilizes Gaussian processes to metamodel the involved biomechanical model.

Semi-explicit discretization of poroelastic equations

Robert Altmann (OvGU Magdeburg)

In this talk, we discuss the time discretization of poroelasticity, a coupled elliptic-parabolic PDE. Fully implicit methods exhibit inefficiency due to the high dimensionality of the coupled problem. As such, we consider a semi-explicit approach, meaning that the mechanics and the flow equations are solved sequentially. In contrast to classical iterative methods such as the well-known fixed-stress scheme, no relaxation parameter or inner iteration is needed. On the other hand, the semi-explicit approach restricts the class of possible applications due to stability issues. To overcome this problem, we

present a novel time integration approach which combines the iterative idea with the semi-explicit Euler approach. For this, we are able to prove first-order convergence for an a priori specified number of inner iteration steps, only depending on the coupling strength.

Modified exponential Rosenbrock methods to increase their accuracy

Begoña Cano (Universidad de Valladolid), María Jesús Moreta

A technique will be described to avoid order reduction with exponential Rosenbrock methods when integrating initial boundary value problems with time-dependent boundary conditions. That requires to calculate some information on the boundary from the given data. We have proved that, under some assumptions on the coefficients of the method which are mainly always satisfied, no numerical differentiation is required to approximate that information in order to achieve order 4 for parabolic problems with Dirichlet boundary conditions. With Robin/Neumann ones, just numerical differentiation in time may be necessary for order 4, but none for order ≤ 3. Furthermore, as with this technique it is not necessary to impose any stiff order conditions, in search of efficiency, we recommend some methods of classical orders 2, 3 and 4 and some comparisons with several methods in the literature, with the corresponding stiff order, will be shown.

Towards the efficient simulation of spatially non-local PDE models on time-dependent spatial domains

Alf Gerisch (TU Darmstadt, Research Group Numerical Analysis and Scientific Computing)

The spatially non-local modelling of attractive and repulsive behaviour of cellular populations has gained considerable popularity and lead to the development of many integro-PDE models. Efficient numerical techniques in one, two, or three space dimensions are available allowing for the simulation of and also the parameter estimation in these models. However, when modelling processes in embryology, these often take place on a time scale in which the embryo is growing considerably as well. This leads to a current interest in integro-PDE models on time-dependent (growing) spatial domains.

Here we are concerned with adapting an existing finite-volume spatial discretization to the case of a time-dependent spatial domain. We focus on a spatially one-dimensional situation as this is sufficient for our initial application in mathematical biology. In this case but also in general the non-local term requires particular attention. In the case of a fixed spatial domain pre-computation and FFT-techniques can be applied in its evaluation, in the case of spatially uniform domain change, pre-computation becomes difficult due to a new time-dependence but FFT can still be applied, and in the case of spatially non-uniform domain change also the use of FFT is essentially ruled out. As a consequence, efficient simulations on spatially uniformly and non-uniformly changing domains are currently possible for integro-PDEs in one space dimension and on spatially uniformly changing domains for integro-PDEs in two space dimensions.

Starting Approximations for SIRK Methods Applied to Index 2 DAEs

Joseph R. Small (University of Iowa (AMCS)), Laurent O. Jay, Juan I. Montijano, Quentin Chediak

Implicit Runge-Kutta (IRK) methods are often used to numerically approximate solutions of stiff differential equations and differential-algebraic equations (DAEs). While these methods have very useful properties that their explicit counterparts lack, they also come at the cost of having to solve a nonlinear system of equations at every time step. In this presentation, we look at applications of IRK methods to index 2 DAEs ($y = f(t, y, z)$, $0 = g(t, y)$), henceforth referred to as specialized implicit Runge-Kutta (SIRK) methods. We are particularly interested in developing high order starting approximations for the internal stages to minimize the number of fixed-point/Newton type iterations needed to solve the nonlinear system within the desired error bounds.

Starting approximations for some of these SIRK methods have been previously studied but our new formulation greatly simplifies the analysis and further-generalizes the methods for which we can apply the approximations. We expand our starting approximations and exact internal stages (in step size h) about the current time-step rather than the previous time-step by using reverse SIRK Methods. Many of these so-called reverse methods had not been considered for index 2 DAEs before this work. Reverse SIRK methods

also have many convenient relationships to the original SIRK methods they stem from, such as satisfying the same simplifying assumptions.
Our starting approximations are split into two parts: The y components and the z components. Both use linear combinations of the previous step's internal stages, while the starting approximations for Y_i's also include the previous and current time-steps. For methods satisfying the simplifying assumption $C(q)$, we are able to develop starting approximations of order q for Y_i's and order $min(q, s-1)$ for Z_i's. The coefficients for these methods are found by solving a linear system dependent on the underlying IRK coefficients.

Bicausal optimal transport for SDEs with irregular coefficients

Michaela Szölgyenyi (University of Klagenfurt, Department of Statistics), Benjamin A. Robinson

We solve an optimal transport problem under probabilistic constraints, where the marginals are laws of solutions of stochastic differential equations with irregular, that is non-globally Lipschitz continuous coefficients. Numerical methods are employed as a theoretical tool to bound the adapted Wasserstein distance. This opens the door for computing the adapted Wasserstein distance in a simple way.

Structure-preserving dynamical model order reduction of parametric Hamiltonian systems

Cecilia Pagliantini (University of Pisa)

In real-time and many-query simulations of parametric differential equations, computational methods need to face high computational costs to provide sufficiently accurate and stable numerical solutions. To address this issue, model order reduction aims at constructing low-complexity high-fidelity surrogate models that allow rapid and accurate solutions under parameter variation. In this talk, we consider the model order reduction of parametric Hamiltonian dynamical systems describing non-dissipative phenomena. The development of reduced order models of such systems is challenged by several factors: (i) failing to preserve the geometric structure encoding the physical properties of the dynamics might lead to instabilities and unphysical behaviors of the

resulting approximate solutions; (ii) the local low-dimensional properties of non-dissipative phenomena demands large reduced spaces to achieve sufficiently accurate approximations; and (iii) nonlinear operators require hyper-reduction techniques that preserve the gradient structure of the flow velocity. We will discuss how to address these aspects via a nonlinear model order reduction approach based on evolving low-dimensional surrogate models on a phase space that adapts in time while being endowed with the geometric structure of the full model.

Solution of hyperbolic problems on cut cell meshes

Sandra May (Department of Information Technology, Uppsala University), Gunnar Birke, Marsha Berger, Christian Engwer, Fabian Laakmann, Florian Streitbürger, Ferdinand Thein, Andreas Westhoff

Cut cells methods have been developed in recent years for computing flow around bodies with complex geometries. For mesh generation, the flow body is cut out of a regular Cartesian grid resulting in so called *cut cells*. Cut cells can have irregular shape and can become arbitrarily small. For the solution of time-dependent hyperbolic conservation laws, this causes the *small cell problem*: explicit time stepping schemes are not stable on the arbitrarily small cut cells.
In this talk, we first illustrate the small cell problem from different perspectives and then give an overview over some existing solution approaches from the literature. We then present two solution approaches, the *mixed explicit implicit scheme* and the *DoD stabilization*, in more detail.
The mixed explicit implicit scheme has been developed in the context of finite volume schemes and is based on treating cut cells fully implicit for stability while using explicit time stepping away from the embedded boundary. The Domain of Dependence (DoD) stabilization has been developed in the context of DG schemes. The stabilization is based on adding suitable penalty terms to the spatial discretization. In time, one can then use a standard explicit time stepping scheme. The terms are designed to restore proper domains of dependence.

Numerical preservation of stochastic dissipativity

Helena Biščević (Gran Sasso Science Institute), Raffaele D'Ambrosio, Stefano Di Giovacchino

Standard numerical analysis for stochastic differential equations has a clear understanding of stability in the linear case or when the drift coefficient satisfies a one-sided Lipschitz condition and the diffusion term is globally Lipschitz. By looking at many applications, it is obvious that we need a deeper mathematical and numerical insight into stability of problems with non-global Lipschitz coefficients.
This talk is aimed to analyze nonlinear stability properties of θ-methods for stochastic differential equations under non-global Lipschitz conditions on the coefficients. In particular, the concept of exponential mean-square contractivity is introduced for the exact dynamics; additionally, stepsize restrictions in order to inherit the contractive behaviour over the discretized dynamics are also given. A selection of numerical tests confirming the theoretical expectations is also presented.
Moreover, we will briefly tackle current work concerning numerical dissipativity for stochastic partial differential equations.

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Transition from conventional computational multibody dynamics approaches to machine learning based methods

Johannes Gerstmayr (University of Innsbruck), Peter Manzl

Dynamic simulations of flexible multibody systems, particularly those involving index 3 constraints, nonlinearities, or discontinuities, remain challenging. In practice, highly heterogeneous system setups, which typically include a mix of rigid and flexible bodies, finite element meshes with modal reduction, hydraulics, and control systems, integrated with external software components, preclude the straightforward application of state-of-the-art GPU acceleration techniques.

This talk commences with the open-source multibody dynamics simulator Exudyn, designed to manage such heterogeneity. While our system attempts to align with the capabilities of both open source and commercial software in the field, it also incorporates Lie-group integrators and automatic differentiation to maintain a lean code. We will discuss the system's design, its limitations, and the performance improvements achieved through traditional multi-threaded parallelization.

For further performance improvements, we have explored potential enhancements using machine learning methods aimed at replicating the input-output behavior of damped multibody systems without detailed knowledge of the states or initial conditions. We employ specially designed feed-forward neural networks, trained on randomized simulations within the expected range of inputs, to predict outputs with accuracy adequate for practical applications. An additional error estimator, trained across an extended range of

inputs, helps to assess the reliability of these predictions. We will present results from several multibody models, demonstrating the accuracy of our predictions and estimators, as well as significant speed improvements over conventional simulations.
Looking ahead, we will discuss the potential for leveraging large language models to generate simulation models based solely on textual descriptions, allowing future engineers to abandon the usage of classical graphical user interfaces and struggles with solver settings.

Modelling relaxation source terms in two-phase flows

Ward Haegeman (ONERA / École polytechnique), Marc Massot, Giuseppe Orlando, Clément Le Touze, Joël Dupays

Compressible two-phase flows occur in several natural phenomena and are of interest for many industrial applications (impinging jets, jet atomizations,...). The Baer-Nunziato multi-fluid model allows to accurately model these flows. The model allows the phases to be out of thermo-mechanical equilibrium and is endowed with relaxation sources terms driving the system towards equilibrium. A hierarchy of sub-models has been derived assuming some of the relaxation processes to be infinitely fast. This has also given rise to several numerical strategies where the hyperbolic part of the system and the relaxation source terms are split. After the hyperbolic step, the relaxation terms are then applied in the limit of instantaneous relaxations, effectively turning them into projection operators on some equilibrium manifold.
In this talk, we will discuss the different instantaneous relaxation processes and analyse the resulting numerical schemes. Main focus will be given to instantaneous pressure relaxations for which effect of the relaxation parameters on the convergence and stability of the schemes will be detailed, these results will then be compared to instantaneous pressure-temperature relaxation schemes.

Principles of geometric numerical integration for stochastic differential equations

Raffaele D'Ambrosio (University of L'Aquila - Department of Information Engineering and Computer Science and Mathematics)

This talk aims to outline some recent advances on structure-preserving numerical methods for stochastic differential equations, highlighting the basic principles of the so-called geometric numerical integration by its history. The talk moves towards the following two tracks:

- *track 1: geometric numerical integration of stochastic Hamiltonian problems.* For these problems, two different scenarios are clarified: if the noise is driven in the Ito sense, the expected Hamiltonian function exhibits a linear drift in time; in the Stratonovich case, the Hamiltonian is pathwise preserved. In both cases, the talk aims to highlight the attitude of selected numerical methods in preserving the aforementioned behaviors. A long term investigation via backward error analysis is also presented;

- *track 2: structure-preserving numerics of stochastic PDEs.* In this case, the attention is focused on the stochastic Korteweg-de Vries equation, characterized by certain invariance laws for the exact dynamics. The talk focuses on their long-term conservation along the numerical dynamics provided by stochastic θ-methods for the time integration of the spatially discretized system.

For all tracks, numerical evidence supporting the theoretical inspection will be provided. The investigation of above tracks is based on the joint research in collaboration with Chuchu Chen (Chinese Academy of Sciences), David Cohen (Chalmers University of Technology & University of Gothenburg), Stefano Di Giovacchino and Annika Lang (Chalmers University of Technology & University of Gothenburg).

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Pathwise methods for a class of SDEs with non-globally Lipschitz coefficients

Hugo de la Cruz (School of Applied Mathematics. FGV EMAp), Mario Munoz

We propose an approach for the numerical integration of a class of multiplicative-noise SDEs with non-globally Lipschitz coefficients. For this, me devise an appropriate invertible continuous transformation, that allows to conjugate the flow of the SDE to the flow of a non-autonomous random differential equation which has the stationary Ornstein-Uhlenbeck process as the only input parameter of the system. In this way, based on this explicit conjugacy between both equations, new discrete-time approximations are constructed. Convergence results are presented, and some simulation studies are carried out to illustrate the practical performance of the introduced approach.

A new approach to construct higher weak order stochastic Runge-Kutta methods

Kristian Debrabant (University of Southern Denmark, Department of Mathematics and Computer Science), Anne Kværnø, Adrien Laurent

The difficulty of the creation of weak high order integrators for stochastic dynamics lies in the tedious calculations of order conditions. The original approaches focused on adapting strong approximations, mainly replacing the iterated stochastic integrals by random variables that have the same moments. The methods obtained this way are sub-optimal in their number of function evaluations.

In this talk, using a specific set of random Runge-Kutta coefficients, we greatly reduce the number of order conditions for weak second order integration of stochastic dynamics. The approach is successfully applied to the creation of a collection of new simple stochastic Runge-Kutta methods of weak order two with an optimal number of stages.

A comparison of different positivity-preserving time integration schemes.

Stefan Kopecz (University of Kassel, Institute of Mathematics), Hendrik Ranocha

Over the last two decades several approaches have been suggested to numerically preserve the positivity of solutions of positive ODE systems. However, a fair comparison of the different schemes has not yet been made.
For this reason, we are developing PositiveIntegrators.jl [1], a Julia package designed to provide efficient implementations of various positive time integration methods. The current focus is on modified Patankar–Runge–Kutta schemes, but many other methods will follow. In addition, PositiveIntegrators.jl extends Julia's standard ODE package OrdinaryDiffEq.jl, which makes it possible to compare the methods of both packages.
In the talk, we will present the current status of the package and show first comparisons of the available methods.

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Randomized low-rank Runge-Kutta methods

Daniel Kressner (EPFL), Hysan Lam

Low-rank integrators, such as dynamical and projected low-rank methods, have been developed to efficiently address differential equations with matrix or tensor valued solutions. Application areas that have benefitted from these

developments include plasma physics, quantum systems and, most recently, machine learning. During the last decade, randomized methods, such as the randomized SVD, have shown their benefits when performing low-rank approximations of (constant) matrices, to the extent that they are now considered a state-of-the-art approach. The purpose of this talk is to carry over these randomized techniques to time-dependent problems. In particular, we will present and analyze a new class of randomized low-rank Runge-Kutta methods. Building mainly on random sketches, these methods are efficient and flexible to exploit different types of sparsity in the data. Theoretical results suggest and numerical experiments validate that these methods can attain arbitrarily high order, which is not always the case for existing low-rank integrators, and perform well for typical benchmark examples of dynamical low-rank methods.

Methods for Domain Preservation

Gabriel Lord (Radboud University), Utku Erdogan

Many stochastic (partial) differential equations that arise, for example in mathematical biology preserve a particular doamin. There are often physical/biological constraints for this such as concentrations should be positive or solutions should lie in a certain domain (eg [0,1] for stochastic gating variables). The question then arises how to preserve these domains in a numerical simulation. We develop a numerical method based on exponential integrators that naturally preserve such domains and discuss convergence and efficiency. This work is joint with Utku Erdogan.

Poisson dynamics: Simulation and Learning

David Martín de Diego (ICMAT, Spain), M. Vaquero, A. Cabrera

In this talk, we will present a method to construct geometric integrators for general nonlinear Poisson manifolds, i.e., numerical methods that preserve the underlying Poisson geometry. Finally, for a particular class of Poisson systems we will show how to approximate the solutions using machine learning techniques.

A multi-index Monte Carlo exponential integrator method for semilinear SPDEs

Andreas Petersson (Linnaeus University), Håkon Hoel (University of Oslo), Abdul-Lateef Haji-Ali (Heriot-Watt University)

The multi-index Monte Carlo method (MIMC) is an extension of the multilevel Monte Carlo method (MLMC). MLMC improves the efficiency of Monte Carlo methods applied to forward uncertainty quantification for stochastic equations by considering a hierarchical sampling on a sequence of levels. MIMC replaces the levels by a vector of indices and may improve the efficiency further. In this ongoing project, we show that MIMC outperforms MLMC when applied to parabolic stochastic PDEs (SPDEs). This holds provided that the discretization scheme of the SPDE has a high second-order difference decay rate. We show that this property is attained by the accelerated exponential Euler scheme of Jentzen and Kloeden. The results hold for a semilinear SPDE with a sufficiently smooth Nemytskij type non-linearity in the drift and with affine linear space-time noise of Itô type.

Evolution equations with a positive memory term in adaptation to the composite finite element framework

Tamal Pramanick (National Institute of Technology (NIT) Calicut), Anjaly Anand

This article discusses the adaptation and convergence analysis by addressing an evolution equation employing the composite finite element method (abbreviated as CFE), incorporating a positive-type memory term. The CFE method is one modification of the standard finite element method (FEM). The benefit of this approach lies in its usage of the two-scale discretization across the domain- one with coarse scale grid size H, the other with fine scale grid size h. This helps in reducing the dimension of the considered domain space. This article examines an initial-boundary value problem involving an integro-differential equation of the Volterra type and we check the convergence using the proposed method. The memory term is a convolution product of an elliptic operator and the positive definite kernel. We discuss the fully discrete estimation for the error analysis, where both the time and space coordinates gets discretized. It is noted that the results obtained are

optimal. We have carried out the numerical experiments for the validation of the theoretical results.
Keywords: Composite finite element method, Parabolic problems, Positive-type memory, Error estimation, Convergnce.
MSC numbers: 65M60, 65N30, 35K58, 65M50, 65M55

Equivalent systems for differential equations with polynomially distributed delays

Roland Pulch (Universität Greifswald, Institut für Mathematik und Informatik)

We consider a delay differential equation (DDE) of the form

$$y'(t) = f\Big(y(t), \int_I y(t-\tau)\, g(\tau)\, \mathrm{d}\tau\Big),$$

which includes a distributed delay in a bounded interval $I = [\tau_{\min}, \tau_{\max}] \subset [0, \infty)$ or an unbounded interval $I = [0, \infty)$. The mapping $g : I \to \mathbb{R}_0^+$ represents a probability density function associated to some probability distribution. In the case of $I = [0, \infty)$ and using a gamma distribution, it is well known that an equivalent system of ordinary differential equations (ODEs) can be arranged. We investigate the case of a bounded interval I and a polynomial g. Important instances are a uniform distribution (g constant) and a beta distribution. We derive an equivalent system, which consists of DDEs including two discrete delays. The properties of this equivalent system are analysed. For comparison, Gaussian quadrature yields a discretisation of the integral in the original DDE. This approach implies a DDE with multiple discrete delays, whose solution approximates the solution of the DDE with distributed delay. We present results of numerical computations, where initial value problems are solved.

Solving a class of singularly perturbed parabolic problems using a new hybrid block method with variable stepsizes

Mufutau Ajani Rufai (Free University of Bozen-Bolzano), Bruno Carpentieri, Higinio Ramos

This presentation will introduce a variable stepsize formulation of a new hybrid block method that efficiently solves a particular class of singularly perturbed parabolic convection-diffusion of partial differential equations using large integration intervals. A theoretical analysis of the new method will be conducted to understand its basic properties. The proposed method will also be implemented in an adaptive mode by adjusting the number and position of nodes used in the approximation to ensure that the truncation error is kept within a specified bound. Based on reasonable error estimation and adaptive strategy that will be presented in this talk, the reliability and accuracy of the introduced method will be observed. Finally, various real-world singularly perturbed parabolic convection-diffusion problems from engineering and scientific domains will be numerically solved to assess the effectiveness and efficiency of the proposed block method.

Alternative perspectives on data

Jennifer Ryan (KTH Royal Institute of Technology)

In this talk alternative approaches to looking at data are discussed. First, data can be viewed in the context of numerical approximations. Secondly, for data with a regular structure, utilising a multi-resolution analysis perspective can allow for sparse representation, accurate detection of discontinuities, and representation of multi+scale physics. While the ability to move data from fine resolutions to coarser resolutions is straight forward utilizing a multi-resolution analysis framework, moving data from a coarse resolution to a finer resolution while reducing errors is more challenging. This relies on incorporating filtering techniques into the multi-resolution analysis framework. This approach has the further advantage of requiring fewer computations to gain insight into calculations such as for Bohm speed [Picklo et al. JCP 2024]. In this talk, we present methods for data enhancement through multi-resolution analysis and the Smoothness-Increasing Accuracy-Conserving (SIAC) filtering framework.

From formulation to implementation in multi-physics simulations

Radu Serban (University of Wisconsin-Madison), Dan Negrut

A multiphysics package for mechanical and mechatronic systems must address and mitigate several factors, often conflicting. These stem from the need to couple significantly different physics, with different formulations and underlying dynamics and hence with different numerical model embodiments and performance and parallelization needs. A general purpose multiphysics software package must be able to simulate vastly different systems, from a watch mechanism, to suspended flow in biological systems, to mobility of heavy tracked vehicles on deformable terrain, to extraterrestrial rovers in low gravity. The breadth of such applications often requires different formulations (e.g., for rigid frictional contact, flexible multibody systems, terramechanics, etc.). In turn, these different formulations lead to different requirements in terms of numerical methods and, ultimately, to different implementation paradigms regarding the most appropriate parallelization techniques and targeted hardware.
We begin by introducing the open-source Chrono multiphysics package and highlighting some of its capabilities and applications. A design and architectural goal of Chrono has been a unified API and modeling and simulation approach, while managing the diversity in formulations and applications.
We then focus on the problem of vehicle-terrain interaction, as a prototypical multiphysics problem, to illustrate some of the above observations and provide details on the design decisions that go from formulation, to software architecture, and to implementation. We discuss aspects related to the choice of contact formulation (smooth vs. non-smooth), terramechanics formulation (empirical, discrete, continuous), software architecture (template-based design vs. one-shot modeling), as well as addressing scale and performance issues in large scale GPU-based granular dynamics.

Port-Hamiltonian modelling and simulation of network DAEs

Caren Tischendorf (Humboldt University of Berlin), Jan Giesselmann, Jonas Pade

We present a port-Hamiltonian modeling of gas networks in form of a partial differential algebraic equation system based on the mass flow balance equation and network element models describing the relation between enthalpy and mass flow. The set of network elements includes pipes, compressors, resistors and valves. We use the pipe model description from [1] that provides perturbation bounds via relative energy estimates.

Using the mixed-finite element spatial discretization part from the pipe discretization presented [2], we derive a port-Hamiltonian differential algebraic equation system. Finally, we present convergence criteria for a waveform relaxation approach for couplings of the resulting network DAEs exploiting the convergence result for coupled DAEs given in [3, Theorem 2.4].

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Numerical analysis of the bouncing ball on the elastic beam

Katarina Tutić (University of Rijeka, Faculty of Civil Engineering), Teo Mudrić, Nina Čeh, Martin Arnold

Modeling non-smooth mechanical systems with unilateral constraints presents significant challenges, particularly in accurately representing contact dynamics and handling velocity discontinuities. This research investigates a dynamic scenario involving a ball bouncing on a deformable beam, illustrating the complexity of contact interactions between rigid and deformable bodies. In this study, the deformable beam is modeled using the finite element method, while the contact interactions are resolved using the Moreau–Jean method [1]. This time-stepping approach maintains a constant time step during simulations, making it particularly effective for systems with frequent contacts. It offers greater efficiency and accuracy compared to event-driven schemes that require very small time steps to handle frequent contact events. Special attention is dedicated to analyzing the effects of different beam stiffness values to precisely evaluate their influence on system dynamics. Additionally, the research investigates how variations in Newton's coefficient of

restitution influence the overall behavior of the system. The study also addresses numerical damping phenomena that arise during simulations when employing the Moreau–Jean method, providing a comprehensive understanding of its implications on the accuracy and stability of the results.

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Relational Inference On Graphs Using Nonlinear Opinion Dynamics

Yulong Yang (Princeton University), Bowen Feng, Kevin Wang, Naomi Leonard, Adji Bousso Dieng, Christine Allen-Blanchette

From pedestrians to Kuramoto oscillators, interactions between agents govern how a multitude of dynamical systems evolve in space and time. Discovering how these agents relate to each other can improve our understanding of the often complex dynamics that underlie these systems. Recent works learn to categorize relationships between agents based on observations of their physical behavior. These approaches are limited in that the relationship categories are modeled as independent and mutually exclusive, when in real world systems categories are often interacting. In this work, we introduce a level of abstraction between the physical behavior of agents and the categories that define their behavior. To do this, we learn a mapping from the agents' states to their affinities for each category in a graph neural network. We integrate the physical proximity of agents and their affinities in a nonlinear opinion dynamics model which provides a mechanism to identify mutually exclusive categories, predict an agent's evolution in time, and control an agent's behavior. We demonstrate the utility of our model for learning interpretable categories for mechanical systems, and demonstrate its efficacy on several long-horizon trajectory prediction benchmarks where we consistently out perform existing methods.

Space-time parallel parareal methods for the solution of parabolic problems

Laura Portero (Public University of Navarre), Iñigo Jimenez, Andres Arraras, Francisco J. Gaspar

Many phenomena in science and engineering are governed by evolutionary partial differential equations. In scenarios involving three-dimensional models or long-term simulations, the computational workload can become a significant bottleneck in achieving fast and accurate solutions. To fully leverage the computational power of modern parallel clusters, extensive research is underway in the area of space-time parallel methods. In this talk, we propose an approach that combines the parallel-in-time parareal algorithm with various time-splitting schemes, enabling spatial parallelization. We will explore both dimensional and domain decomposition partitioning strategies for solving parabolic problems. A key advantage of these methods is that both the fine and coarse propagators operate in parallel, in contrast to the classical parareal algorithm, where all processors remain idle during coarse propagator computations. This approach uses parallel computational cores for both integrators, significantly enhancing efficiency. We provide a convergence analysis of the proposed methods and present several numerical experiments to evaluate the performance of the solvers.

Exact Integration for Rational Finite Elements

Johannes Storn (Universität Leipzig), Tabea Tscherpel, Lars Diening

This talk summarizes a joint work with Tabea Tscherpel and Lars Diening. We introduce an exact integration formula for a class of rational polynomials in 2D. Based on this we present finite element implementations using rational basis functions. In particular, we present simple Matlab implementations of the singular Zienkiewicz and the lowest-order Guzman–Neilan Element.

Explicit-Implicit Domain Splitting for Two Phase Flows with Phase Transition

Ferdinand Thein (Johannes Gutenberg-Universität Mainz), Sandra May

Two phase flows that include phase transition, especially phase creation, with a sharp interface remain a challenging task for numerics. In this talk, we present recent results for the isothermal Euler equations with phase transition between a liquid and a vapor phase, see [1]. The phase interface is modeled as a sharp interface and the mass transfer across the phase boundary is modeled by a kinetic relation. Using sharp interfaces for simulating nucleation and cavitation results in the grid containing tiny cells that are several orders of magnitude smaller than the remaining grid cells. This forces explicit time stepping schemes to take tiny time steps on these cells. To overcome this issue we propose an explicit implicit domain splitting where only the neighborhood of the tiny cells is treated implicitly. We use dual time stepping to solve the resulting small implicit systems. Our numerical results indicate that the new scheme is robust and provides significant speed-up compared to a fully explicit treatment

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A general class of multirate Runge-Kutta methods for coupled atmosphere-ocean models

Tobias Bauer (Federal Agency for Cartography and Geodesy)

Coupled atmosphere-ocean models are applied for studying physical processes at the air-sea interface. The exchange at the air-sea interface, i.e. at the coupling interface, is conducted in each integration step. However, to reduce computational and energy costs for large simulations, individual time steps are used for the atmosphere and ocean part. The exchange at the air-sea interface is then conducted either with the large time step of the slow ocean component or with an even larger individual time step.
Multirate Runge-Kutta methods are an approach for efficient integration of differential equations with different time scales. The main idea of multirate approaches is the splitting or partitioning of a problem into several time

scaled parts. The simplest splitting type is a linear combination.
A general formulation of a class of multirate Runge-Kutta methods is presented which can be applied to split problems with an arbitrary number of additive parts. This class of methods also allows different time scales for each part, with no restrictions on the choice of time scales.
Furthermore, a method for a problem split into three parts is developed and presented as well as illustrated with a simulation of a coupled atmosphere-ocean model.

Structure preserving neural network-based learning Euler*'s elastica and constitutive model discovery for myocardium*

Sigrid Leyendecker (Institute of Applied Dynamics, Friedrich-Alexander-Universität Erlangen-Nürnberg), Denisa Martonová, Martina Stavole

In the context of structure preserving neural network-based learning methods, two approaches are presented in the mechanical setting: approximation of Euler's elastica used for modelling of flexible endoscopes, and automated constitutive model discovery for human myocardium. We demonstrate that we can successfully train the networks, on the one hand, to preserve structural invariants, like e.g. the inextensibility constraint of the predicted trajectories [1], and, on the other hand, to satisfy thermodynamic consistency of the myocardial stress-strain behaviour [2].
Starting from a data set of solutions of the discretised static equilibria of Euler's elastica in [1], the neural networks is trained to produce trajectories – firstly as continuous functions ('continuous networks') and secondly in terms of discrete configurations ('discrete network') – for unseen boundary conditions. Different ways to ensure the inextensibility constraint are considered in the supervised learning. The continuous networks preserve the structure of the problem by construction or by incorporating the constraint into the loss function. Even though the discrete neural network does not include structural information in its design or loss, it predicts trajectories accurately satisfying the inextensibility constraint.
In [2], instead of selecting a specific constitutive model a priori and fitting its parameters to data, we utilise *constitutive neural networks* preserving physically motivated constraints. The network autonomously discovers the best model and parameters to characterise the constitutive behavior of the

passive human myocardium. We demonstrate that we can successfully train the network with triaxial shear and biaxial extension tests and systematically sparsify the parameter vector with L_1-regularization. Further, we show that the discovered model outperforms popular existing myocardium models and generalises well, from homogeneous laboratory tests to heterogeneous whole heart simulations.

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Gaussian Process

Hazem Yaghi (TU Braunschweig)

A Gaussian Process (GP) is a stochastic process over space or time that, when restricted to a finite number of points, yields a collection of jointly Gaussian random variables. It is considered as a probabilistic supervised machine learning technique that can be applied widely in regression and classification tasks.
In this talk we illustrate the surrogate modeling capabilities of GPs in different scenarios. In the project SEMOTI we introduce a surrogate modeling approach for a deep geological repository based on GPs. The surrogate model is used as a substitute for the mechanical model in many-query scenarios, such as parameter identification.
On other hand we apply GPs to find an approximate solution for a scalar hyperbolic conservation law with uncertainty.

Structure-preserving methods for simulation and learning of dynamical systems

Kathrin Flaßkamp (Saarland University)

The classical approach to predicting behavior of dynamical systems is to treat the mathematical modeling and the numerical integration as subsequent steps. Contrarily, structure-preserving methods, as they have been developed particularly for mechanical systems, intertwine them to generate discrete-time models, still based on first-principle modeling. Motivated by the growing interest in machine learning, we revisit these methods to study the potential of data-based enhancements.
This presentation gives insight into three aspects of this endeavor: Firstly, Hamiltonian neural networks which preserve and learn unknown system invariances, namely affine-linear Lie group symmetries, are introduced for system identification. Secondly, we present AI-enhanced symplectic numerical integrators which allow a structure-preserving efficiency increase. Lastly, we consider dynamical control systems possessing symmetry-induced relative equilibria, known as motion primitives. These primitives can be extracted from data as we demonstrate in an autonomous driving application.

On tight stepsize restrictions for monotonicity and positivity of Runge-Kutta methods

Inmaculada Higueras (Public University of Navarre), Teo Roldan

We consider differential problems whose solutions have qualitative properties that are relevant in the context of the problem. When these problems are solved numerically, the preservation of these qualitative properties is crucial to obtain physically meaningful numerical solutions. Strong Stability Preservation (SSP) theory can be used to obtain time step bounds that ensure this preservation. However, it is well known that, for many problems, the stepsize restrictions obtained with this approach are not sharp, and some robust non-SSP methods performs well. Sharper step size restrictions can be obtained by taking into account the structure of the differential problem. In this talk, we show some results on the numerical preservation of monotonicity and positivity of Runge-Kutta methods for some classes of problems.

Advanced Exponential and Multirate Integrators for Multiple Time Scale Problems

Luan Vu Thai (Texas Tech University, Department of Mathematics and Statistics)

Many science and engineering problems involve multiple physical processes, with complex interactions that result in dynamics spanning a wide range of time scales. This presents significant challenges for real-time simulation of these multiphysics problems. A prominent example is the existence of vastly differing time scales in atmospheric phenomena, ranging from a relatively slow advection to very fast gravity waves, which poses significant difficulties for real-time simulation of weather and long-term climate predictions. Developing fast and accurate time integration methods is thus crucial for a wide range of applications that rely on simulations of complex multiphysics systems.
In this talk, we will present our recent advancements in constructing, analyzing, and implementing new exponential and multirate time integration methods. These methods enhance both accuracy and efficiency in computational simulations of large-scale, multiple time scale problems. We will also showcase their performance through numerical experiments across various applications, including visual computing, numerical weather prediction, and computational biology.

Learning efficient and provably convergent splitting methods

Henry Lockyer (University of Bath), L. M. Kreusser, E. H. Müller, and P. Singh

Splitting methods are widely used for solving initial value problems (IVPs) due to their ability to simplify complicated evolutions into more manageable subproblems. These subproblems can be solved efficiently and accurately, leveraging properties like linearity, sparsity and reduced stiffness. Traditionally, these methods are derived using analytic and algebraic techniques from numerical analysis, including truncated Taylor series and their Lie algebraic analogue, the Baker–Campbell–Hausdorff formula. These tools enable the development of high-order numerical methods that provide exceptional accuracy for small timesteps. Moreover, these methods often (nearly) conserve

important physical invariants, such as mass, unitarity, and energy. However, in many practical applications the computational resources are limited. Thus, it is crucial to identify methods that achieve the best accuracy within a fixed computational budget, which might require taking relatively large time steps. In this regime, high-order methods derived with traditional methods often exhibit large errors since they are designed to be asymptotically optimal. Machine Learning techniques offer a potential solution since they can be trained to efficiently solve a given IVP for large timesteps, but they are often purely data-driven, come with limited convergence guarantees in the small-timestep regime and do not necessarily conserve physical invariants. In this work, we propose a framework for finding machine learned splitting methods that are computationally efficient for large time steps and have provable convergence and conservation guarantees in the small-timestep limit.

Crossroads between Geometric Numerical Integration and Machine Learning

Michael Kraus (Max-Planck-Institut für Plasmaphysik)

Many dynamical systems in physics and other fields possess some form of geometric structure, such as Lagrangian or Hamiltonian structure, symmetries and conservation laws. Geometric numerical integration algorithms which preserve these structures usually show greatly reduced errors and better long-time stability compared to algorithms that do not preserve these structures. In this talk, we will show how the ideas of geometric numerical integration can be brought forward to the realms of scientific machine learning, where neural networks are used to solve differential equations.

Investigation of isothermal Baer-Nunziato-type models

Siegfried Müller (RWTH Aachen University, Institut für Geometrie und Praktische Mathematik), Maren Hantke, Aleksey Sikstel, Ferdinand Thein

Compressible multi-component flows where the fluid is a mixture of several components all of which may be present in different aggregate states have a wide range of applications, for instance a mixture of reacting gases or a mixture of a liquid and a gas. They have been successfully modeled by

Baer-Nunziato-type models, see for instance [4]. In recent years, work on barotropic Baer-Nunziatio models has been published in [3, 1, 5].
The main interest is on multi-component Baer-Nunziato-type models for mixtures with an arbitrary number of components all of which are modeled by immiscible isothermal fluids. These are given by balance equations for volume fractions, density and momentum for each component accounting for the relaxation to equilibrium by means of relaxation terms. In the talk the Baer-Nunziato model for isothermal flows is derived from the full Baer-Nunziato model, see [4], taking into account the heat flux.
Thermodynamical consisteny of the model is verified. For this purpose, first an appropriate Lax' entropy-entropy flux pair is derived where, in particular, the phasic energy equations including the heat flux is accounted for, see [4]. Furthermore, to ensure an entropy equality appropriate interfacial pressures and interfacial velocity are chosen. In particular, unique interfacial pressures are determined depending on the interfacial velocity chosen as a convex combination of the phasic velocities. By this, the Baer-Nunziato models are closed.
Finally, instantaneous relaxation to equilibrium is investigated and appropriate algorithms are presented. These are used to perform numerical computations using a path-conservative DG scheme. Details on the presentation can be found in the preprint [2].

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Learning of Lagrangian dynamics from data with uncertainty quantification

Christian Offen (Paderborn University)

I will show how to use Gaussian Process regression to learn variational dynamical systems from data. From the statistical framework uncertainty quantification for observables such as the Euler-Lagrange operator and Hamiltonians can be derived. The regression method can be shown to converge, overcoming the technical difficulty that variational descriptions are highly non-unique. Numerical examples include variational odes and pdes.

Positive invariance and strong stability preservation of SVD and POD for time-stepping methods

Zoltán Horváth (Széchenyi István University, Győr)

Model reduction is necessary for solving time-dependent problems with millions or billion state variables per time-step, which is the case e.g. when solving large-scale environmental or industrial applications. The proper orthogonal decomposition (POD) and its variants have been used by several solutions. The POD consists of offline generation of snapshots and the singular value decomposition (SVD) is used for defining projections to a low-rank space. SVD gives the L2-optimal projector. It is not obvious what will POD do with the invariance preservation properties (e.g. positivity, total variation diminishing, strong stability).
In this talk, we present an invariance-preserving theorem for the POD time-stepping. We prove that if the snapshot matrix is generated from invariance-preserving data, then the projected flow does preserve the invariance property whenever the initial state is within a smaller invariance set and the singular values decrease at least at a prescribed rate. For this theorem we shall prove an invariance preservation property of the low-rank approximations by the SVD.

Approximation of the Navier-Stokes-Cahn-Hilliard System for Incompressible Two-phase Flows

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In this project we consider the dynamics of two incompressible and immiscible fluids in the convection-dominated regime at constant temperature. For the interfacial dynamics we employ a diffuse-interface approach. The Navier-Stokes-Cahn-Hilliard (NSCH) system is widely used to model the evolution of interfaces in two-phase flows. However, the fourth-order differential operator in the NSCH system results in high computational costs. Therefore, we focus on the NSCH system in a different way and suggest a low-order approximation. The incompressible NS equations are used with artificial compressibility such that the Euler-part of the NS equations is converted to a first-order system. Then, the CH equation is approximated by the Euler-Korteweg (EK) system with friction. It has been proved in (Lattanzio & Tzavaras, 2017) that solutions of the EK system with friction converge to solutions of the CH equation in the limit of infinite friction. Finally, the NS system and the EK system with friction are coupled in a thermodynamically consistent way. By applying a relaxation approach for third-order derivatives in the coupled system, we obtain a first-order system (neglecting the viscosity term). The aim of coupling is to obtain a first-order hyperbolic system of equations. To analyze the hyperbolicity of the new system, the eigenvalues of the Jacobian of the flux are computed. The characteristic analysis of the coupled system shows that it is strictly hyperbolic. Having a hyperbolic system of equations allows us to use tailored numerical methods. In order to solve the new system we use a high-order discontinuous Galerkin method. Finally, numerical experiments for merging droplets are performed with the first-order hyperbolic system and compared to corresponding results of the original NSCH system.