6th Workshop
on
Stability and Discretization Issues in Differential Equations

June 7-10, 2022

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List of speakers

- Fruzsina Agócs
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- Anne Kværnø
- Stefano Maset
- Alexander Ostermann
- Gustaf Söderlind
- Raul Tempone
- Yen-Hsi Richard Tsai
- Ewa Weinmüller

Venue

Eötvös Loránd University, Faculty of Science

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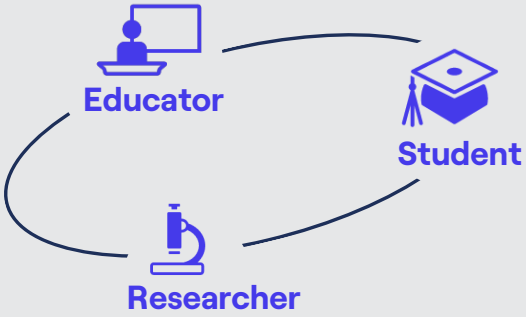

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Schedule of the workshop

Tuesday, 7 June	**Wednesday, 8 June**	**Thursday, 9 June**	**Friday, 10 June**
8.00 *Registration*			
9.00 *Opening*	9.00 Ascher	9.00 Tempone	9.00 Ostermann
9.30 Ketcheson	9.30 Einkemmer	9.30 Kværnø	9.30 Hadjimichael
10.00 Karátson	10.00 R. Horváth	10.00 M. Kovács	10.00 Z. Horváth
10.30 *Coffee break*	10.30 *Coffee break*	10.30 *Coffee break*	10.30 *Closing Coffee*
11.00 B. Kovács	11.00 Cohen	11.00 Söderlind	
11.30 Auzinger	11.30 Debrabant	11.30 Izzo	
12.00 Dörich	12.00 Kelly	12.00 Maset	
12.30 *Lunch*	12.30 *Lunch*	12.30 *Lunch*	
14.00 Agócs	14.00 Conte	11.00 Tsai	
14.30 Kropielnicka	14.30 Weinmüller	14.30 Forberger	
15.00 *Coffee break*	15.00 *Coffee break*	15.00 *Coffee break*	
Working groups	*Working groups*	15.30 - 17.00 GAMAX Presentation and training	

Abstracts of the talks

FAST AND ACCURATE NUMERICAL SOLVERS FOR OSCILLATORY ODES

Fruzsina Julia Agocs

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Oscillatory systems are ubiquitous in physics: they arise in celestial and quantum mechanics, electrical circuits, molecular dynamics, and beyond. Yet even in the simplest case, when the frequency of oscillations changes slowly but is large, the vast majority of numerical methods struggle to solve such equations. Methods based on approximating the solution with polynomials are forced to take $\mathcal{O}(k)$ timesteps, where k is the characteristic frequency of oscillations. This scaling can generate unacceptable computational costs when the ODE in question needs to be solved billions of times, e.g. as the forward modelling step of Bayesian parameter estimation.
In this talk I will introduce a novel set of efficient methods for solving 2nd order, linear ODEs with highly oscillatory solutions.
I will present `(py)oscode` [1, 2, 3], an open-source Python/C++ package that can automatically switch between two different methods to advance the numerical solution with depending on whether the solution is oscillatory or slowly varying. In regions of oscillation it uses an asymptotic expansion (the Wentzel–Kramers–Brillouin approximation) suited for oscillatory functions and can thus step over many oscillations in a single time-step, otherwise switching to a Runge–Kutta method. This allows the number of timesteps `(py)oscode` needs to take to be roughly $\mathcal{O}(1)$, independent of the frequency k. I will briefly summarise the algorithm underlying `(py)oscode` and show examples of its applications, including finding the eigenvalues of a quantum system and the rapid computation of primordial power spectra for exploring models of cosmic inflation. I will compare `(py)oscode` to existing numerical methods for oscillatory systems and discuss its limitations. Finally, I will introduce another (work-in-progress) numerical method built loosely on the ideas behind `(py)oscode`, which was designed to be efficient even at extremely low tolerances approaching machine precision.

References

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STABLE SIMULATION OF DEFORMABLE OBJECTS FOR COMPUTER ANIMATION

Uri M. Ascher

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We examine a variety of numerical methods that arise when considering dynamical systems in the context of physics-based simulations of deformable objects. Such problems arise in various applications, including animation, robotics, control and fabrication. The goals and merits of suitable numerical algorithms for these applications are different from those of typical numerical analysis research in dynamical systems. Here the mathematical model is not fixed a priori but must be adjusted as necessary to capture the desired behaviour, with an emphasis on effectively producing lively animations of objects with complex geometries. Results are often judged by how realistic they appear to observers as well as by the efficacy of the numerical procedures employed. Maintaining stability without over-damping becomes a major challenge. We show that with an adjusted view numerical analysis and applied mathematics can contribute significantly to the development of appropriate methods and their analysis in a variety of areas including finite element methods, stiff and highly oscillatory ODEs, model reduction, and constrained optimization. Please see [1].

References

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ADAPTIVE TIME PROPAGATION OF THE MCTDHF EQUATIONS

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We compare exponential-type integrators for the numerical time-propagation of the equations of motion arising in the multiconfiguration time-dependent Hartree–Fock method (MCTDHF) for solving the high-dimensional multi-particle Schrödinger equation.

We find that among the most widely used integrators like Runge–Kutta, exponential splitting, exponential Runge–Kutta, exponential multistep and Lawson methods, exponential Lawson multistep methods with predictor/corrector step provide optimal stability and accuracy at the least computational cost, taking into account that the evaluation of the nonlocal potential terms is by far the computationally most expensive part of such a calculation.

Moreover, the corrector step provides an estimator for the time-stepping error at no additional cost, which enables adaptive time-stepping to reliably control the accuracy of a computation.

References

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SPLITTING INTEGRATORS FOR STOCHASTIC LIE–POISSON SYSTEMS

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We present explicit stochastic Poisson integrators, based on a splitting strategy, for a class of stochastic Poisson systems driven by Stratonovich noise. We analyse their qualitative and quantitative properties: preservation of Casimir functions as well as strong and weak rates of convergence. Illustrations of these properties for stochastically perturbed Maxwell–Bloch, rigid body and sine–Euler equations will be provided.

The presentation is based on a joint work with C-E. Bréhier and T. Jahnke.

TIME-ACCURATE AND HIGHLY-STABLE EXPLICIT NUMERICAL METHODS FOR DIFFERENTIAL PROBLEMS

Dajana Conte

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This talk concerns the efficient and stable numerical solution of stiff initial value problems of the type

$$\begin{cases} y'(t) = f\Big(t, y(t)\Big), \\ y(t_0) = y_0, \end{cases} \qquad f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d, \quad t \in [t_0, T], \tag{1}$$

also arising in the semi-discretization in space of partial differential equations with advection or diffusion terms. We consider two-step s-stage explicit parallelizable peer methods of the form [4]

$$\begin{aligned} Y_{n,i} &= \sum_{j=1}^{s} b_{ij} Y_{n-1,j} + h \sum_{j=1}^{s} a_{ij} f(t_{n-1,j}, Y_{n-1,j}), \\ Y_{n,i} &\approx y(t_{n,i}), \quad t_{n,i} = t_n + hc_i, \quad 1 \leqslant 1 \leqslant s, \end{aligned} \tag{2}$$

where $\{t_n = t_0 + nh, n = 0, ..., N, t_N = T\}$ is a fixed uniform grid. The solution at the grid points is computed by means of the last stage $Y_{n,s}$, then selecting $c_s = 1$.
To improve the stability of the considered methods (2), Jacobian dependent peer methods have been introduced in [3]. We propose in this talk a further improvement by employing a recently introduced numerical technique, which consists of multiplying the vector field f of (1) by an operator, called Time-Accurate and Highly-Stable Explicit (TASE) operator [1]. New TASE peer methods are obtained by applying peer methods (2) to the resulting modified problem. It is shown that A-stable two-stage order-two and A(θ)-stable three-stage order-three TASE peer methods can be obtained [2]. Finally, numerical tests confirming the efficiency of the derived methods are carried out.
The presented research has been conducted in collaboration with Giovanni Pagano and Beatrice Paternoster, from the Department of Mathematics of the University of Salerno.

References

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LAWSON SCHEMES FOR STOCHASTIC DIFFERENTIAL EQUATIONS

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In this talk, we consider the application of stochastic Lawson schemes to the numerical of stochastic differential equations (SDEs)

$$\mathrm{d}X(t) = \sum_{m=0}^{M} (A_m X(t) + g_m(t, X(t))) \star \mathrm{d}W_m(t), \quad X(t_0) = X_0, \tag{3}$$

where W_m for $m = 1, \dots, M$ denote independent scalar Wiener processes, $W_0(t) = t$ denotes the time, the SDE is solved on the interval $I = [t_0, T]$ and we also assume that the matrices $A_m \in \mathbb{R}^{d\times d}$, $m = 0, \dots, M$, are constant and are chosen in connection with g_m such that the following commutativity assumption holds:

$$[A_l, A_k] = A_l A_k - A_k A_l = 0 \qquad \text{for all} \qquad l, k = 0, 1, \dots, M.$$

We discuss inheritance of the convergence properties of the underlying Runge–Kutta scheme and are especially interested in stochastic midpoint and trapezoidal Lawson schemes and their ability to preserve quadratic invariants.
Details of the analysis can be found in [1, 2].

References

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EXPONENTIAL INTEGRATORS FOR QUASILINEAR WAVE-TYPE EQUATIONS

Benjamin Dörich, Marlis Hochbruck

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In this talk we propose two exponential integrators of first and second order applied to quasilinear hyperbolic evolution equations. We work in an analytical framework which is an extension of the classical Kato framework and covers quasilinear Maxwell's equations in full space and on a smooth domain as well as a class of quasilinear wave equations.
In contrast to earlier works, we do not assume regularity of the solution but only on the data. From this we deduce a well-posedness result upon which we base our error analysis. Turning to the space and full discretization of quasilinear problems, lower bounds on the polynomial degree or severe CFL-type conditions have to be imposed in order to guarantee well-posedness of the numerical method. We complement the talk indicating recent results achieved in [2] towards the full discretization of quasilinear wave equations with improved CFL conditions.

Acknowledgments Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 258734477 – SFB 1173.

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SOME STABILITY RESULTS FOR EXPLICIT DYNAMICAL LOW-RANK INTEGRATORS

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When solving high-dimensional partial differential equations the number of degrees of freedom scales very unfavorable with the dimensions. For a d dimensional problem and n grid points in each direction we require n^d degrees of freedom. This is often referred to as the curse of dimensionality and for $d > 3$ is usually the most challenging aspect in designing efficient numerical methods.
While there is a plethora of complexity reduction techniques that in some situations can alleviate the curse of dimensionality, they usually rely on smoothness and thus do not work reliably for hyperbolic problems. In recent years dynamical low-rank integrators have received significant interest. Numerical simulation show that for many problems (ranging from plasma physics [3] and radiative transfer to uncertainty quantification in fluid dynamics [4]) this approach allows us to drastically reduce the number of degrees of freedom required to obtain an accurate simulation.
However, while it is known that explicit time integrators in combination with a dynamical low-rank approximation can result in reduced stability for hyperbolic problems, there are few mathematical results available. This is due to the fact even a linear equation results in a nonlinear set of equations once the dynamical low-rank approximation has been performed. In this talk we will report on a recently conducted stability analysis for dynamical low-rank algorithms in combination with explicit time integrators [1]. This allows us to explain the CFL condition observed in numerical simulations and in particular emphasizes the good behavior with regards to stability of the recently proposed unconventional integrator [2].

References

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SOLVING ORDINARY DIFFERENTIAL EQUATIONS USING NEURAL NETWORKS

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Not all differential equations have a closed-form solution. To find approximate solutions to these types of equations, many traditional numerical algorithms are available. However, you can also solve an ODE by using a neural network. This approach comes with several advantages, including that it provides differentiable approximate solutions in a closed analytic form.
This includes a neural network containing the weights. Hence by construction the initial/boundary conditions are satisfied and the network is trained to satisfy the differential equation. The useable range starts from ordinary differential equations (ODE) to systems of coupled ODE and also to partial differential equations (PDE). In this presentation I will illustrate the method by solving ODE problems and training an augmented neural ordinary differential equation (ODE) network. A neural ODE is a deep learning operation that returns the solution of an ODE. In particular, given an input, a neural ODE operation outputs the numerical solution of the ODE. An augmented neural ODE operation improves upon a standard neural ODE by augmenting the input data with extra channels and then discarding the augmentation after the neural ODE operation. Empirically, augmented neural ODEs are more stable, generalize better, and have a lower computational cost than neural ODE [1].
The example presented shows you how to:

- generate training data in the given range,
- define a neural network that takes x as input and returns the approximate solution to the ODE,
- train the network with a custom loss function,
- compare the network predictions with the analytic solution.

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HIGH ORDER STRONG-STABILITY-PRESERVING RUNGE–KUTTA METHODS WITH DOWNWIND-BIASED OPERATORS

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Strong stability preserving (SSP) time integrators have been developed to preserve certain nonlinear stability properties (e.g., monotonicity, boundedness) of the numerical solution in arbitrary norms, when coupled with suitable spatial discretizations. The existing general linear methods (including Runge-Kutta and linear multistep methods) either attain small time steps for strong stability preservation or are only first-order accurate. One way to increase the time-step restrictions is to consider time integrators that contain both upwind- and downwind-biased operators.

In this talk, we review SSP Runge-Kutta methods that use upwind- and downwind-biased discretizations in the framework of perturbations of Runge-Kutta methods. We show how downwinding improves the SSP properties of time-stepping methods and breaks some order barriers. In particular, we focus on implicit downwind SSP Runge-Kutta methods that their SSP coefficient can vary with respect to the method's coefficients. We present a novel one-parameter family of third-order, three-stage perturbed Runge-Kutta methods, for which the CFL-like step-size restriction can be arbitrarily large. The stability of this family of methods is analyzed, and we demonstrate that the desired order of accuracy is obtained for large CFL numbers. Furthermore, we discuss the complexity of solving the nonlinear problem that occurs at each step and we propose a block factorization that enhances the solution of Newton's method.

ON SOME OSCILLATORY PROPERTIES OF FINITE DIFFERENCE METHODS FOR ONE-DIMENSIONAL NONLINEAR PARABOLIC PROBLEMS

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In this talk, we investigate two special qualitative properties of the finite difference solutions of one-dimensional nonlinear parabolic initial boundary value problems. The first property says that the number of the sign-changes of the solution function must be non-increasing in time. The second property requires a similar property for the number of the local maximizers and minimizers. First we recall and formulate some theorems that guarantee the above properties for the solution of a special second order nonlinear parabolic problem. Then we generate the numerical solution with the finite difference method and give sufficient conditions for the mesh size and the time step that guarantee the discrete versions of the properties. We also give some numerical test results.

Acknowledgments This research was supported by the Hungarian Scientific Research Fund OTKA, No. K137699 and SNN125119.
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STRONG STABILITY AND POSITIVE INVARIANCE PRESERVATION OF DIAGONALLY IMPLICIT TIME-STEPPINGS IN BANACH SPACES

Zoltán Horváth and Tihamér A. Kocsis

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In this paper, we shall present *IE-cond*, a brand new condition under which strong stability preservation (SSP) will be proved for diagonally implicit time-stepping methods for initial value problems in Banach spaces. The *IE-cond* condition is a statement on the SSP property for the Implicit Euler method. This condition is in general much weaker than the state-of-the-art *EE-cond* condition for the SSP-property with the Explicit Euler method, introduced and thoroughly analyzed by Shu and Osher, S. Gottlieb, Spijker, Kraaijevanger, and many authors. More precisely, *EE-cond* implies *IE-cond*, and *IE-cond* holds true and computable for several problems of practical interest (e.g. non-lumped finite element discretization and/or higher-order semi-discretization of parabolic and hyperbolic problems) for which *EE-cond* does not hold.

In the paper, under the *IE-cond*, we prove SSP-theorems on diagonally implicit time-steppings, based on the results on linear and non-linear resolvents, and methods of convex analysis. Analog properties to the *EE-cond*-based classical theorems will be proved. In addition, optimal diagonally implicit Runge-Kutta methods will be computed up to order 4. It is interesting that for order $p = 4$ there are significant differences between the *IE-cond*-optimal and *EE-cond*-optimal schemes. Similar to the SSP-property, forward invariance preservation of convex sets will be analyzed and theorems proved under the *IE-cond* for positive invariance.

A new, efficient implementation procedure of the diagonally implicit methods will be derived from the new theory.

To illustrate the new theoretical findings, we shall present the results of computational experiments for finite element methods with FEniCS.

AN OVERVIEW ON SELF STARTING GENERAL LINEAR METHODS

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We have recently focused our attention on using general linear methods (GLMs) as a framework to analyze and generalize existing classes of numerical methods for ordinary differential equations. In this work we present the class of Self Starting GLMs, whose name point out one of their main features. Indeed, although they are multi-stage multi-step methods, they do not require any additional starting procedure. In particular, after presenting the general formulation, we focus on a subclass with a structure that is very similar to Runge-Kutta methods. With this approach, we show how some properties of these last methods can be improved, keeping similar computational costs. This analysis indicates that the proposed methods may have better accuracy and stability properties, such as, for example, larger stability regions in the case of explicit methods, or stage order greater than one for singly diagonally implicit methods.
The possibility of identifying good families of methods with a larger number of degrees of freedom can also have implications in the field of time discretization of partial differential equations. For example, Self Starting GLMs allow the determination of new efficient and highly stable Implicit-Explicit methods.
Finally, we report numerical experiments which confirm that Self Starting GLMs are competitive with Runge-Kutta methods and can have better performance on nonstiff, mildly stiff and stiff problems.

Part of this work is joint with Zdzislaw Jackiewicz, Arizona State University (USA), and Sebastiano Boscarino, University of Catania (Italy).

QUALITATIVE PROPERTIES FOR NONLINEAR PARABOLIC FINITE ELEMENT PROBLEMS

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For a given numerical method, besides its convergence, it is also important that the numerical solution shall preserve the characteristic properties of the modeled phenomenon. This ensures the qualitative reliability of the method. For diffusion type parabolic partial differential equations (PDEs), the most relevant such properties are

- maximum/minimum principles,
- in particular, nonnegativity/nonpositivity preservation,
- maximum norm contractivity.

For instance, violation of nonnegativity would often mean that the obtained numerical solution contradicts basic physical laws.

In this talk we summarize some qualitative results related to nonlinear parabolic operators of the following form on a bounded spatial domain:

$$\mathcal{N}[u] \equiv \frac{\partial u}{\partial t} - \operatorname{div}\Big(K(x,t,\nabla u)\Big) + q(x,t,u) \tag{4}$$

with proper nonlinear coefficients. First we deal with the continuous case (operator level), then we study analogous properties for finite element discretizations. The preservation of the qualitative properties can be generally guaranteed with angle conditions on the space mesh (see [1] on the elliptic case) and additional relations of the space mesh and the time-step. Discrete nonnegativity preservation and maximum principles will be summarized for a class of parabolic problems. Furthermore, it is also important to reveal the relations of the involved qualitative properties in an organized network. The results are mainly based on [3, 4], which extend the properties of the linear case in [2].

Acknowledgments This work has been carried out in collaboration with István Faragó, Róbert Horváth and Sergey Korotov. The author is grateful for the support of the Scientific Funds BME NC TKP2020 grant of NKFIH Hungary, and of the Hungarian Scientific Research Fund OTKA (grants SNN125119 and K 137699).

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AN ADAPTIVE SPLITTING METHOD FOR THE COX-INGERSOLL-ROSS PROCESS

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The Cox-Ingersoll-Ross (CIR) process is described by an Itô-type stochastic differential equation with a square-root diffusion and appears frequently in financial applications, for example in the pricing of interest rate derivatives (see [1]):

$$dX(t) = \kappa\left(\theta - X(t)\right)dt + \sigma\sqrt{X(t)}dW(t), \qquad X(0) = X_0 > 0, \tag{5}$$

Solutions of (5) are almost surely (a.s.) non-negative; in fact when $2\kappa\theta > \sigma^2$, a parameter constraint called Feller's condition, they are known to be a.s. positive. For Monte Carlo estimates, exact sampling from the conditional distribution is possible but computationally inefficient, and potentially restrictive if the innovating Brownian motion is correlated with that of another process.

The challenge for numerical methods is to control error in spite of the unbounded gradient of the diffusion near zero, and to preserve the domain invariance of sampled trajectories. As a consequence the numerical simulation of (5) is an active topic of research, and techniques to handle the unbounded gradient of the diffusion coefficient near zero can be applied to more general equations.

We propose a domain invariant numerical method for (5) applied over both deterministic and adaptive random meshes and based upon a suitable transform followed by a splitting. Moment bounds and theoretical strong L_2 and L_1 convergence rates of order $1/4$ the scheme are available in a restricted parameter regime. We then extend the new method to cover all parameter values by introducing a *soft zero* region (where the deterministic flow determines the approximation) resulting in a hybrid method that deals with the reflecting boundary.

From numerical simulations we observe an optimal convergence rate of 1 within the Feller regime. As σ increases and we move outside of this parameter region, we observe that the rates of strong convergence are competitive with other schemes in terms of convergence order, however the proposed method with adaptive timestepping consistently displays smaller error constants.

Acknowledgments This is joint work with Gabriel Lord, Radboud University, The Netherlands.

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INVARIANT-PRESERVING DISCRETIZATIONS OF DISPERSIVE WAVE EQUATIONS

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Many dispersive wave equations have a Hamiltonian structure, with important conserved quantities of both linear and nonlinear type. The accuracy of over long times of numerical discretizations. depends critically on the preservation of these invariants. I will present a class of invariant-preserving discretizations based on summation-by-parts in space and relaxation in time; these fully-discrete schemes conserve both linear and nonlinear invariants and can be either implicit or explicit. These schemes have been developed for a wide range of such equations, including Benjamin-Bona-Mahony (BBM), Fornberg-Whitham, Camassa-Holm, Degasperis-Procesi, Holm-Hone, and the BBM-BBM system. I will show examples demonstrating that the error for such schemes grows only linearly in time, whereas for general schemes the error grows quadratically. I will also show examples of non-dispersive hyperbolic systems where such invariant-preserving schemes lead to a similar (drastic) improvement in long-time accuracy.

ERROR ESTIMATES FOR BULK–SURFACE SPLITTING METHODS FOR PARABOLIC PROBLEMS WITH DYNAMIC BOUNDARY CONDITIONS

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In this talk we will discuss some interesting convergence results splitting methods for parabolic problems with dynamic boundary conditions. A key property of these splitting methods is that they separate the bulk and boundary dynamics.

The first (naive) bulk–surface splitting methods [KL17] have suffered from order reduction. Recently we proposed two completely different approaches [AKZ22] and [CFK22a] to overcome this issue. In the talk, with the help of numerical experiments, we will discuss and compare these methods and also give some details on their error analysis.

The talk is based on joint work with Robert Altmann and Christoph Zimmer (Augsburg), and Petra Csomós (Rényi & ELTE) and Bálint Farkas (Wuppertal).

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SOME APPROXIMATION RESULTS FOR MILD SOLUTIONS OF STOCHASTIC FRACTIONAL ORDER EVOLUTION EQUATIONS

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We investigate the quality of space approximations of a class of stochastic integral equations of convolution type with Gaussian noise. Such equations arise, for example, when considering mild solutions of stochastic fractional order partial differential equations but also when considering mild solutions of classical stochastic partial differential equations. The key requirement for the equations is a smoothing property of the deterministic evolution operator which is typical in parabolic type problems. We show that if one has access to nonsmooth data estimates for the deterministic error operator together with its derivative of a space discretization procedure, then one obtains error estimates in pathwise Hölder norms with rates that can be read off the deterministic error rates.

This is a joint work with Erika Hausenblas (Montanuniversität Leoben) and Kistosil Fahim (Institut Teknologi Sepuluh Nopember).

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HIGHLY ACCURATE INTEGRATORS FOR THE LINEAR KLEIN-GORDON EQUATIONS FROM LOW TO HIG FREQUENCY REGIMES

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In this talk, we consider the Klein–Gordon equation

$$\begin{cases} \frac{\partial^2}{\partial t^2}\psi(x,t) = \Delta\psi(x,t) - m(x,t)\psi(x,t), \quad t > t_0, \quad x \in \mathbb{T}^d \\ \psi(x,t_0) = \psi_0(x), \quad \partial_t\psi(x,t_0) = \varphi_0(x) \end{cases} \tag{6}$$

equipped with periodic initial and boundary conditions and time and space dependant coefficient $m(x,t)$. The latter assumption was proposed only recently in [1] and allows for dealing with the problems of negative probability density and of violation of Lorenz covariance. Moreover application of time ans space dependant coefficients extends application of (6) to the domain of quantum cosmology, [2], where $m(x,t)$ may bring possibly highly oscillatory form

$$m(x,t) = \sum_n a_n(x,t)e^{i\omega_n t} \tag{7}$$

with frequencies $\omega_n \in \mathbb{R}$, $n \in \mathbb{Z}$.
Numerical approximation of (6) with (7) requires various approaches when $m(x,t)$ is non-oscillatory, or highly oscillatory. The most challenging form of coefficient $m(x,t)$, however, is when it includes low and high frequencies, for example $m(x,t) = a_0(x,t) + a_1(x,t)\mathrm{e}^{it} + a_2(x,t)\mathrm{e}^{i10^6 t}$.
In this talk we will present various approaches to all the kinds of these problems, will present final error estimates and plenty of numerical examples.

Results of these investigations were obtained with Karolina Lademann (University of Gdansk) and Katharina Schratz (Sorbonne Universite).

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A HIGH ORDER EXPONENTIAL INTEGRATOR FOR SEMILINEAR SDES WITH ADDITIV NOISE.

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In this talk, we discuss the numerical solution of a semilinear SDE with additive scalar noise, on the form

$$dX(t) = AX(t)\mathrm{d}t + f(t, X(t))\mathrm{d}t + g(t)\mathrm{d}W(t)$$

where $A \in \mathbb{R}^{d\times d}$ is a constant matrix, and $W(t)$ is a scalar Wiener process.
We will discuss how the order theory for exponential integrators derived in [1] can be simplified and adjusted to the problem in question and present an mean square order 1.5 method based on these conditions.
The method has been applied to a semi-discretized diffusion-reaction PDE with bounday noise, and some implementation issues will be discussed.

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RELATIVE ERRORS IN LINEAR ODEs

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In the integration of the linear ODE

$$\begin{cases} y'(t) = Ay(t), \ t \geqslant 0, \\ y(0) = y_0, \end{cases}$$

we consider the errors due to:

- a perturbation of the initial value y_0;
- a perturbation of the matrix A;
- the use of a numerical method, i.e. the use of an approximant of the matrix exponential.

In the talk, we are interested to the relative errors rather than the absolute errors and we show how these relative errors propagates along the time t. In particular, we are interest to the their long-time behavior.
By looking to the relative errors, we explore an aspect of the numerical ODEs which is little known and new and interesting results arise by this analysis. For example:

- in case of a perturbation of the initial value, unlike the absolute error, the relative error of the perturbed solution does not diverge or decay to zero depending on the real part of the rightmost eigenvalue of A, but it remains bounded and away from zero;
- the relative error of the numerical method grows linearly in time.

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NUMERICAL INTEGRATION OF NLS: NON-SMOOTH DATA ERROR ESTIMATES

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Standard numerical integrators such as splitting methods or exponential integrators suffer from order reduction when applied to semi-linear dispersive problems with non-smooth initial data. In this talk, we focus on the cubic nonlinear Schrödinger equation with periodic boundary conditions. For such problems, we present and analyze (filtered) integrators that exhibit superior convergence rates at low regularity. Numerical examples illustrating the analytic results will be given.

This is joint work with Frédéric Rousset (Paris-Sud) and Katharina Schratz (Sorbonne, Paris).

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ADAPTIVE LINEAR MULTISTEP METHODS: DESIGNING AUTOMATIC STEP SIZE CONTROL FOR MULTISTEP METHODS

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In a k-step adaptive linear multistep methods the coefficients depend on the k-1 most recent step size ratios. In a similar way, both the actual and the estimated local error will depend on these step ratios. The classical error model has been the asymptotic model, $r = ch^{p+1}y^{(p+1)}(t)$, based on a constant step size analysis, where all past step sizes simultaneously go to zero. This does not reflect actual computations with multistep methods, where step size control only affects future steps, not the the previous accepted steps. In variable step size implementations, therefore, even in the asymptotic regime, the error model must include the dependence on previous step sizes and step ratios. In this talk we develop dynamic asymptotic models for variable step size computations, and analyze a new step size controller accounting for the dynamics in the error model, while keeping the local error near a prescribed tolerance.

ADAPTIVE MULTILEVEL MONTE CARLO FOR PDEs AND SDEs

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We will first recall the use of Monte Carlo and Multi-level Monte Carlo (MLMC) methods. Then we will discuss our goal-oriented Multilevel Monte Carlo (AMLMC) algorithms for (i) Partial Differential Equations with random inputs, (ii) Ito Stochastic Differential Equations, and (iii) Stochastic Reaction Networks modeled by Pure Jump Markov Processes. In this context, adaptivity includes several aspects such as mesh refinements based on either a priori or a posteriori error estimates, the local choice of different time-stepping methods, and the selection of the total number of levels and the number of samples at different levels. Our AMLMC estimator uses a hierarchy of adaptively refined, non-uniform discretizations. In particular, we show that our AMLMC algorithms are asymptotically accurate and have the correct complexity using the pointwise convergence of an appropriate error density. We even offer improved control of the multiplicative constant factor in the asymptotic analysis. We then recall our Continuation MLMC algorithm for estimating parameters needed in MLMC, such as the variance of the difference between consecutive approximations. CMLMC takes particular care of the deepest levels, where only a few realizations are available to produce essential estimates for efficiency reasons. Moreover, we show the asymptotic normality of the statistical error in the MLMC estimator, justifying an error estimate that allows prescribing both the required accuracy and confidence level in the final result. We present several examples to illustrate the above results and the corresponding computational savings.

TIME-PARALLEL COMPUTATION OF HAMILTONIAN SYSTEMS AIDED BY MACHINE LEARNING

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We propose a machine learning approach for time-parallel computations of Hamiltonian systems. We will demonstrate the approach by computing wave propagation in media with multiscale wave speeds, using a second-order linear wave equation model as a proof-of-concept. We advocate the use of online- and offline data for enhancing the parareal algorithm of Lions, Maday, and Turinici [1], and demonstrate that the coupled approach improves the stability of parareal algorithms for wave propagation and improves the accuracy of the enhanced coarse solvers [2, 3]. The central focuses are the formulation of an optimization problem and the generation of suitable training data, in other words, the sampling of the appropriate function space. We discuss the regime in which similar machine learning approaches may have computational advantages given appropriate optimization models and data.

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EFFICIENT SOLUTION OF BVPS IN ODES WITH SINGULARITIES

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We deal with boundary value problems for systems of ordinary differential equations with singularities. Typically, such problems have the form

$$z'(t) = F(t, z(t)), \quad t \in (0, 1], \quad B_0 z(0) + B_1 z(1) = \beta,$$

where $\lim_{t\to 0} F(t, z(t)) = \infty$ and $\lim_{t\to 0} \partial F(t, z)/\partial z = \infty$. The analysis is usually done for the model equation

$$z'(t) = \frac{1}{t^\alpha} M z(t) + f(t, z(t)), \quad t \in (0, 1], \quad B_0 z(0) + B_1 z(1) = \beta,$$

where $f(t, z)$ may also be in the form of $g(t, z)/t$ with a smooth function $g(t, z)$. For $\alpha = 1$ the problem has a *singularity of the first kind*, while for $\alpha > 1$ the singularity is commonly referred to as *essential singularity*. We briefly recapitulate the analytical properties of the above problems with a special focus on the most general boundary conditions which guarantee their well-posedness.

To compute the numerical approximation for z we use polynomial collocation, because the method retains its hight order even in case of singularities. The usual high-order superconvergence at the mesh points does not hold in general. However, the uniform superconvergence is preserved (up to logarithmic factors). We will discuss how the collocation performs for problems with the inhomogeneity of the form $g(t, z)/t$.

The updated version of the MATLAB code `bvpsuite1.1` with the special focus on the above problem class has been implemented. For higher efficiency, estimate of the global error and adaptive mesh selection are provided. The code can be applied to arbitrary order problems in implicit form. Also systems of index 1 differential-algebraic equations (DAEs) are in the scope of the code. We illustrate the performance of the software with a special focus on parameter-dependent problems by means of numerical simulation of models in applications.

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