UNIVERSITÀ DEGLI STUDI DI NAPOLI
FEDERICO II

Workshop

Efficient high-order time discretization methods for PDEs

May 11-13, 2022

Villa Orlandi, Anacapri, Italy

Università di Catania

Università degli Studi di Ferrara

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*: *Online participant.*

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Scientific Committee

- **Sebastiano Boscarino,** Dipartimento di Matematica e Informatica, Università degli Studi di Catania, Italy.
- **Giuseppe Izzo**, Dipartimento di Matematica e Applicazioni "R.Caccioppoli", Università degli Studi di Napoli Federico II, Italy.
- **Lorenzo Pareschi**, Dipartimento di Matematica e Informatica, Università degli Studi di Ferrara, Italy.
- **Giovanni Russo**, Dipartimento di Matematica e Informatica, Università degli Studi di Catania, Italy.

Organizing Committee

- **Sebastiano Boscarino,** Dipartimento di Matematica e Informatica, Università degli Studi di Catania, Italy.
- **Giuseppe Izzo**, Dipartimento di Matematica e Applicazioni "R.Caccioppoli", Università degli Studi di Napoli Federico II, Italy.

Invited Talks

Staggered discretisation of the Euler equation: how to achieve local conservation

Rémi Abgrall

University of Zurich, Switzerland

This paper is focused on the approximation of the Euler equation of compressible fluid dynamics on a staggered mesh. To this aim, the flow parameter are described by the velocity, the density and the internal energy. The thermodynamic quantities are described on the elements of the mesh, and this the approximation is only L^2, while the kinematic quantities are globally continuous. The method is general in the sense that the thermodynamical and kinetic parameters are described by arbitrary degree polynomials, in practice the difference between the degrees of the kinematic parameters and the thermodynamical ones is equal to 1. The integration in time is done using a defect correction method. As such, there is no hope that the limit solution, if it exists, will be a weak solution of the problem. In order to guaranty this property, we introduce a general correction method in the spirit of the Lagrangian staggered method described in [1] and [2], and we prove a Lax Wendroff theorem. The proof is valid for multidimensional version of the scheme, though all the numerical illustrations, on classical benchmark problems, are all one dimensional because we have an easy access to the exact solution for comparison. We also provide two dimensional simulations on triangular and quad meshes. We conclude by explanning that the method is general and can be used in a different setting as the specific one used here, for example finite volume, of discontinuous Galerkin methods.

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On the construction of conservative semi-Lagrangian IMEX advection schemes for multiscale time dependent PDEs

Walter Boscheri
University of Ferrara, Italy

This talk is devoted to present the construction of a new class of semi-Lagrangian (SL) schemes with implicit-explicit (IMEX) Runge-Kutta (RK) time stepping for PDEs involving multiple space-time scales. The semi-Lagrangian (SL) approach fully couples the space and time discretization, thus making the use of RK strategies particularly difficult to be combined with. First, a simple scalar advection-diffusion equation is considered as a prototype PDE for the development of a high order formulation of the semi-Lagrangian IMEX algorithms. The advection part of the PDE is discretized explicitly at the aid of a SL technique, while an implicit discretization is employed for the diffusion terms. In this way, an unconditionally stable numerical scheme is obtained, that does not suffer any CFL-type stability restriction on the maximum admissible time step. Second, the SL-IMEX approach is extended to deal with hyperbolic systems with multiple scales, including balance laws, that involve shock waves and other discontinuities. A conservative scheme is then crucial to properly capture the wave propagation speed and thus to locate the discontinuity and the plateau exhibited by the solution. A novel SL technique is proposed, which is based on the integration of the governing equations over the space-time control volume which arises from the motion of each grid point. High order of accuracy is ensured by the usage of IMEX RK schemes combined with a Cauchy-Kowalevskaya procedure that provides a predictor solution within each space-time element. The one-dimensional shallow water equations (SWE) are chosen to validate the new conservative SL-IMEX schemes, where convection and pressure fluxes are treated explicitly and implicitly, respectively. The asymptotic-preserving (AP) property of the novel schemes is also studied considering a relaxation PDE system for the SWE. A large suite of convergence studies for both the non-conservative and the conservative version of the novel class of methods demonstrates that the formal order of accuracy is achieved and numerical evidences about the conservation property are shown. The AP property for the corresponding relaxation system is also investigated.

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Implicit and semi-implicit high-order well-balanced methods for systems of balance laws

Manuel Jesús Castro-Díaz

Universidad de Málaga, Spain

The goal of this work is to design implicit and semi-implicit high-order well-balanced numerical methods for systems of balance laws with stiff numerical flux and source term. Here we use the general strategy introduced by Castro-Pares (2020) to construct high-order well-balanced reconstruction operators that are combined with standard RK-IMEX or RK-Implicit to integrate in time the balance laws. We will show that strategy that we propose is able to maintain the properties of the RK-IMEX and RK-implicit method design for the homogenous system and the well-balanced property of the reconstruction operator, ensuring the well-balanced character of the resulting methods. This general strategy will be applied to several systems of balance laws, such as the Burgers equation with source term or the 1D shallow water system.

Discrete conservation laws for finite element discretisations of multisymplectic PDEs

Elena Celledoni

Norwegian University of Science and Technology, Norway

We propose a new, arbitrary order space-time finite element discretisation for Hamiltonian PDEs in multisymplectic formulation. We show that the new method which is obtained by using both continuous and discontinuous discretisations in space, admits a local and global conservation law of energy. We also show existence and uniqueness of solutions of the discrete equations. Further, we illustrate the error behaviour and the conservation properties of the proposed discretisation in extensive numerical experiments on the linear and nonlinear wave equation and the nonlinear Schrödinger equation.

On the treatment of curl involutions in Newtonian continuum mechanics and general relativity

Michael Dumbser

University of Trento, Italy

In this talk we present several first order hyperbolic PDE models from Newtonian continuum mechanics and from general relativity that are endowed with curl constraints. In particular, we consider the recent first order hyperbolic system of compressible multi-phase flows with surface tension proposed by Gavrilyuk et al., the first order hyperbolic reformulation of the nonlinear defocusing Schrödinger equation and a new first order hyperbolic reformulation of the Einstein field equations of general relativity (FO-CCZ4). In all cases, evolution equations for auxiliary gradient fields are added to the original PDE system, leading to the natural constraint that the curl of the auxiliary field must remain zero for all times if it was initially zero. In many cases, the resulting first order hyperbolic system is only weakly hyperbolic, which poses several challenges from a numerical point of view. In this talk we present a novel generalization of the successful generalized Lagragian multiplier (GLM) approach of Munz et al. to the treatment of PDE with curl constraints. The proposed GLM curl cleaning approach is conservative and allows to restore strong hyperbolicity of the system. We show several numerical examples in the context of Newtonian mechanics and in general relativity.

High order strong stability preserving multi-derivative implicit and IMEX Runge-Kutta methods

Sigal Gottlieb

University of Massachusetts Dartmouth, USA

In this talk we present a class of high order unconditionally strong stability preserving (SSP) implicit two-derivative Runge-Kutta schemes, and SSP implicit-explicit (IMEX) multi-derivative Runge-Kutta schemes where the time-step restriction is independent of the stiff term. The unconditional SSP property for a method of order $p > 2$ is unique among SSP methods, and depends on a backward-in-time assumption on the derivative of the operator. We show that this backward derivative condition is satisfied in many relevant cases where SSP IMEX schemes are desired. We devise unconditionally SSP implicit Runge-Kutta schemes of order up to $p = 4$, and IMEX Runge-Kutta schemes of order up to $p = 3$. For the multi-derivative IMEX schemes, we also derive and present the order conditions, which have not appeared previously. The unconditional SSP condition ensures that these methods are positivity preserving, and we present sufficient conditions under which such methods are also asymptotic preserving when applied to a range of problems, including a hyperbolic relaxation system, the Broadwell model, and the Bhatnagar-Gross-Krook (BGK) kinetic equation.

Joint work with Zachary Grant, Jingwei Hu, *and* Ruiwen Shu.

Quantum algorithms for computing observables of nonlinear partial differential equations

Shi Jin

Shanghai Jiao Tong University, China

Nonlinear partial differential equations (PDEs) are crucial to modelling important problems in science but they are computationally expensive and suffer from the curse of dimensionality. Since quantum algorithms have the potential to resolve the curse of dimensionality in certain instances, some quantum algorithms for nonlinear PDEs have been developed. However, they are fundamentally bound either to weak nonlinearities, valid to only short times, or display no quantum advantage. We construct new quantum algorithms - based on level sets - for nonlinear Hamilton-Jacobi and scalar hyperbolic PDEs that can be performed with quantum advantages on various critical numerical parameters, even for computing the physical observables, for arbitrary nonlinearity and are valid globally in time. These PDEs are important for many applications like optimal control, machine learning, semi-classical limit of Schrodinger equations, mean-field games and many more. Depending on the details of the initial data, it can display up to exponential advantage in both the dimension of the PDE and the error in computing its observables. For general nonlinear PDEs, quantum advantage with respect to M, for computing the ensemble averages of solutions corresponding to M different initial data, is possible in the large M limit.

Joint work with Nana Liu.

Convergence and error analysis for multidimensional Euler equations

Mária Lukácová-Medvidová
University of Mainz, Germany

In this talk I will present our recent results on the convergence analysis of some finite volume and higher order discontinuous Galerkin methods applied to the Euler equations in two- and three-space dimensions. In general, we obtain only weak* convergence to a generalized, dissipative measure-valued solution. If the classical solution exists, the dissipative measure-valued solutions coincide with the classical solution and the convergence of numerical solutions is strong. In this case we can also derive the error estimates. To this end we combine the consistency errors with the continuous form of the relative energy inequality. This allows us to measure an error between a numerical solution and an exact classical solution. Our approach is general and can be applied to any consistent numerical method.

The present research has been done in collaboration with Eduard Feireisl, Bangwei She *and* Philipp Öffner. *It has been supported by the Gutenberg Research College and Mainz Institute of Multiscale Modeling.*

Stability of Modified Patankar-Runge-Kutta Methods

Andreas Meister
University of Kassel, Germany

The talk mainly focuses on stability statements of modified Patankar-Runge-Kutta (MPRK) methods, which have proven to be efficient and robust numerical schemes that preserve positivity and conservativity of production-destruction system irrespectively of the time step size chosen. Due to these advantageous properties they are used for a wide variety of applications. Beside a fundamental introduction of MPRK(α) as well as MPRKncs(α) methods, the center manifold theory is used in order to investigate the Lyapunov stability of general positive and conservative time integrator schemes. Based on the derived results, we prove that MPRK22(α) schemes are unconditionally stable and derive the stability regions of MPRK22ncs(α) methods. Finally, numerical experiments will be presented, which confirm the theoretical results and show the performance of MPRK schemes in comparison with standard Runge-Kutta methods when applied to advection-diffusion-reaction systems.

Joint work with Stefan Kopecz and Thomas Izgin (University of Kassel, Germany).

Some ideas for large time steps to integrate balance laws

Gabriella Puppo
Università di Roma La Sapienza, Italy

In recent years we have witnessed a large body of research concentrated on Low Mach problems. The idea is that in many applications propagation phenomena induced by hyperbolic systems are characterized by very different speeds, while the phenomenon of interest is carried by low speed waves. In gas dynamics this typically occurs in almost incompressible flow, where the acoustic waves are much faster than material waves. In these cases, the classical CFL condition of explicit schemes forces small time steps, even though one is really interested in the advection of material waves. In this talk I will describe the issues behind the construction of Low Mach schemes, and a few solutions on which I have worked. I will consider both intrusive schemes, exploiting deeply the structure of the equations, and relaxed schemes which promise a more general approach. I think that this approach is interesting, because most if not all Low Mach schemes are problem-specific. Applications will be shown to elastic materials and multiphase flows. Finally, I will conclude with the description of a scheme we are proposing which is a sort of black box high order implicit scheme for hyperbolic problems.

Explicit-implicit-null (EIN) time-marching for high order PDEs

Chi-Whang Shu
Brown University, USA

Time discretization is an important issue for time-dependent partial differential equations (PDEs). For the k-th (k is at least 2) order PDEs, the explicit time-marching method may suffer from a severe time step restriction $\tau = O(h^k)$ (where τ and h are the time step size and spatial mesh size respectively) for stability. The implicit and implicit-explicit (IMEX) time-marching methods can overcome this constraint. However, for the equations with nonlinear high derivative terms, the IMEX methods are not good choices either, since a nonlinear algebraic system must be solved (e.g. by Newton iteration) at each time step. The explicit-implicit-null (EIN) time-marching method is designed to cope with the above mentioned shortcomings. The basic idea of the EIN method is to add and subtract a sufficiently large linear highest derivative term on one side of the considered equation, and then apply the IMEX time-marching method to the equivalent equation. The EIN method so designed does not need any nonlinear iterative solver, and the severe time step restriction for explicit methods can be removed. Coupled with the EIN time-marching method, we will discuss high order finite difference and local discontinuous Galerkin schemes for solving high order dissipative and dispersive equations. For simplified equations with constant coefficients, we perform analysis to guide the choice of the coefficient for the added and subtracted highest order derivative terms in order to guarantee stability for large time steps. Numerical experiments show that the proposed schemes are stable and can achieve optimal orders of accuracy for both one-dimensional and two-dimensional linear and nonlinear equations.

This talk is based on joint work with Haijin Wang, Qiang Zhang *and* Shiping Wang, *and with* Meiqi Tan *and* Juan Cheng.

Contributed Talks

Multi-scale modeling and numerics of Sorption Kinetics

Clarissa Astuto

King Abdullah University of Science & Technology, Saudi Arabia

The trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of different real problems in chemistry, physics and biology [1]. Here we study the dynamics of diffusing particles in a domain with a spherical trap-bubble.

We investigate the correlated motion between positive and negative ions exposed to the attraction of a bubble surface that mimics the (oscillating) cell membrane [2]. The correlated diffusion of surfactants is described by a Poisson-Nernst-Planck (PNP) system, in which the drift term is given by the gradient of a potential which includes both the effect of the bubble and the Coulomb interaction between the carriers. The latter term is obtained from the solution of a self-consistent Poisson equation. For very short Debye lengths one can adopt the so called Quasi-Neutral limit which drastically simplifies the system, thus allowing for much faster numerical simulations. We present a PNP model that describes ion charges in presence of a trap. Then we explore the validity of the Quasi-Neutral limit by comparison with detailed numerical simulation for smaller and smaller Debye lengths. In order to reach these goals, we propose a simple and efficient Alternate Direction Implicit method for the numerical solution of the non-linear PNP system, which guarantees second order accuracy both in space and time, without requiring solution of nonlinear equation at each time step.

In the second part of the talk, we propose and validate a multiscale model for the description of particle diffusion in presence of trapping boundaries [3]. We start from a drift-diffusion equation in which the drift term describes the effect of bubble traps. The interaction of the particles attracted by the bubble surface is simulated by the Lennard-Jones potential. In our model the effect of the potential is replaced by a suitable boundary condition derived by mass conservation and asymptotic analysis. The potential is assumed to have a range of small size ε. An asymptotic expansion in the ε is considered, and the boundary conditions are obtained by retaining the lowest order terms in the expansion.

The validity of the model is carefully checked with several tests in 1D, 2D and different geometries.

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Physics-informed neural networks for multiscale hyperbolic models for the spatial spread of infectious diseases

Giulia Bertaglia

University of Ferrara, Italy

The purpose of this talk is to present some recent results in the mathematical modeling of epidemic phenomena through the use of kinetic equations and their numerical solution with physics-informed machine learning techniques.

When studying real epidemic scenarios, the model parameters, necessary to simulate the predictive dynamics of the propagation of the virus of interest, require a delicate calibration phase, often made even more challenging by the scarcity of observed data reported by official sources. Moreover, one of the main problems in studying the propagation of epidemics consists in the great uncertainty of available data, such as the real number of infected individuals (as demonstrated by the recent COVID-19 pandemic, especially in its early phase). Thus, we are commonly forced to draw conclusions and make decisions having only partial and random information at our disposal.

A class of multiscale hyperbolic transport models is introduced to study the propagation of an infectious disease described by the diffusive behavior characterizing a part of the population acting over an urban scale and the transport mechanism related to individuals traveling in extra-urban scales. Recently developed asymptotic-preserving (AP) physics-informed neural networks (PINNs) for hyperbolic transport models of epidemic spread are designed to solve the inverse and the forward problem of interest without losing the ability to describe the multiscale dynamics of the phenomenon. Given the large uncertainty on epidemic data reported by official sources, noisy and stochastic data are also taken into account. Several numerical experiments are discussed to confirm the validity of the proposed methodology.

This is part of joint works with S. Jin (Shanghai Jiao Tong University), C. Lu (Iowa University), L. Pareschi (University of Ferrara)*, and* X. Zhu (Iowa University).

Semi-Lagrangian IMEX vortex methods

Giacomo Dimarco
University of Ferrara, Italy

In this talk, we discuss the construction of a new class of semi-Lagrangian schemes with implicit-explicit (IMEX) Runge-Kutta (RK) time discretizations for the solution of the incompressible Navier-Stokes equations written in vorticity formulation. Within this formulation, the advection part is discretized explicitly at the aid of a Semi-Lagrangian technique, while an implicit discretization is employed for the diffusion term. Several numerical examples show that the theoretical order of convergence is reached by this class of methods and their capability in accurately solving standard problems arising in incompressible fluid dynamics simulations.

Novel high-resolution semi-implicit finite volume methods for conservation laws

Peter Frolkovič

Slovak University of Technology, Slovakia

In this talk we present recent results on our development of higher order semi-implicit finite volume methods applied to some representative equations of conservation laws. The method can be seen as an extension of the first order accurate implicit method as given, e.g., in [1]. In its simplest form it is based on a partial Cauchy-Kowalevski (or Lax-Wendroff) procedure when the time derivatives in the Taylor series are replaced by mixed derivatives using the PDE [2]. To suppress nonphysical oscillations in numerical solutions, the TVD second order accurate form is derived similarly to [3]. Moreover, first results on the WENO type of semi-implicit finite volume schemes will be presented.

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A computationally efficient strategy for time-fractional diffusion-reaction equations

Roberto Garrappa
Università degli Studi di Bari, Italy

The numerical treatment of diffusion-reaction equations with time-fractional derivatives is often a very challenging task from the computational point of view. The non-locality of fractional-order operators, and the need of considering a persistent memory in the numerical computation, usually result in an extremely demanding need of storage memory and computational resources.

In this work [1] we devise a computationally efficient strategy to perform numerical simulations in an acceptable time and with a reasonable memory occupation. An ImEx product-integration rule is coupled with a kernel compression scheme allowing to approximate the non-local problem in a sequence of local problems. To optimize the computational task involved by solving the large number of local problems, we adopt a matrix form for the semidiscretized problem so as to require the solution of Sylvester equations only with small matrices.

Results about the accuracy of the proposed scheme are presented together with numerical experiments showing the efficiency of this strategy from the computational point of view.

Joint work with Marina Popolizio (Politecnico di Bari, Italy).

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Perturbed Runge-Kutta methods for mixed precision applications

Zachary Grant

Michigan State University, USA

In this work we consider a mixed precision approach to accelerate the implemetation of multi-stage methods. We show that Runge–Kutta methods can be designed so that certain costly intermediate computations can be performed as a lower-precision computation without adversely impacting the accuracy of the overall solution. In particular, a properly designed Runge–Kutta method will damp out the errors committed in the initial stages. This is of particular interest when we consider implicit Runge–Kutta methods. In such cases, the implicit computation of the stage values can be considerably faster if the solution can be of lower precision (or, equivalently, have a lower tolerance). We provide a general theoretical additive framework for designing mixed precision Runge–Kutta methods, and use this framework to derive order conditions for such methods. Next, we show how using this approach allows us to leverage low precision computation of the implicit solver while retaining high precision in the overall method. We present the behavior of some mixed-precision implicit Runge–Kutta methods through numerical studies, and demonstrate how the numerical results match with the theoretical framework. This novel mixed-precision implicit Runge–Kutta framework opens the door to the design of many such methods.

Towards parallel-in-time methods for the moist shallow water equations

Nell Hartney

University of Exeter, UK

Weather and climate forecasting rely heavily on the use of supercomputers to numerically solve the PDEs that describe the evolution of the atmosphere. The changing trend in supercomputer architecture towards massively parallel systems is motivating a redesign of forecasting algorithms to support routes to parallelism. In particular, we are interested in the problem of parallel temporal discretisation of the equations, and are investigating several routes to time parallelism for these PDEs. These include schemes based on exponential integrators, parallelised through the use of a rational approximation which approximates the integral as a sum (the terms of which can be computed in parallel), as well as schemes based on predictor-corrector methods such as integral deferred correction and parareal. A natural starting point in the design of these algorithms is the rotating shallow water equations, which are the usual test bed for atmospheric model development. As a simpler model than the full three-dimensional system the shallow water equations are computationally cheap, but they retain the challenge of timescale separation present in the full equations due to the presence of both slow Rossby waves and faster inertial-gravity waves. The addition of moisture to the system introduces an additional challenge due to the switch-like forcing. I will present an overview of our approach to investigating time-parallel methods for these equations using the Gusto finite element dynamical core toolkit, and show results from recent test cases.

Maximum principle preserving space and time flux limiting

David Ketcheson

King Abdullah University of Science & Technology, Saudi Arabia

I will present a framework for enforcing maximum (or minimum) bounds on the solution of a scalar conservation law including both hyperbolic and diffusive terms. The method can be used to achieve arbitrarily high order accuracy in time and space, thus providing a way to get past the well-known order barriers for SSP time discretizations. The approach is based on combining a high-order almost-bound-preserving solution with a first-order bound-preserving solution through a novel limiting technique. I will show examples using WENO finite volume methods in space and high-order extrapolation Runge-Kutta methods in time. If there is time I will show preliminary results of applying the same technique to preserve positivity for the shallow water equations.

An implicit-explicit strategy for Exner model with Grass Equation for sediment evolution

Emanuele Macca

University of Catania, Italy

The aim of this talk is introduce an Implicit-Explicit (IMEX) strategy to compute the sediment evolution [1, 2] in the Exner model for sediment transport [3] in Shallow Water system and improve both stability and efficiency. In this model there are several time scales. One associated with the temporal evolution of the sediment, generally very long with a much slower velocity; one related to the velocity of free-surface waves, generally very fast that implies an hard restriction in the time step; and one related to the velocity of the fluid with. Unfortu- nately, as known, an explicit method implies a strong stability restriction due to the velocity of the free-surface wave. This restriction involves in a very long computation time that could be reduced neglecting the free-surface waves behaviour and looking at the sediment evolution. The objective is to drastically improve the efficiency in the computation of the evolution of the sediment by treating water waves implicitly, thus allowing much larger time steps than the one allowed by standard CFL condition on explicit schemes.

Joint work with Manuel J. Castro-Diaz (University of Malaga, Spain) *and* Giovanni Russo (University of Catania, Italy).

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Positive and conservative nonstandard schemes for biochemical systems

Angela Martiradonna

University of Bari Aldo Moro, Italy

Many important phenomena in biology, chemistry, epidemiology and ecology are modelled by differential systems with two main qualitative characteristics: positive solutions and conservation of linear invariants, such as the total density. A suitable numerical integrator for these models should therefore be featured by the same two characteristics. In this work [1], we generalize the nonstandard Euler and Heun schemes in order to provide explicit geometric numerical integrators for biochemical systems, here denoted as GeCo schemes, which preserve both positivity of the solutions and linear invariants. We show the performance of GeCo schemes in solving some nonlinear biochemical systems and compare them with similar schemes in literature.

Joint work with Fasma Diele *and* Gianpiero Colonna*, CNR, Italy* .

References

[1] Martiradonna, A., Colonna, G., Diele, F., GeCo: Geometric Conservative nonstandard schemes for biochemical systems. Applied Numerical Mathematics, 155, 38-57 (2020).

Time discontinuous Galerkin methods for wave propagation problems

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The study of direct and inverse wave propagation phenomena is an area of intensive research and finds important applications in different engineering areas including acoustics, aeroacoustics, electromagnetics, and computational seismology. From the mathematical perspective, the physics governing these phenomena can be modeled by means of the wave equation. From the numerical viewpoint, a number of distinguished challenges arise when tackling such kinds of problems, and reflect onto the following features required to the numerical schemes: accuracy, geometric flexibility, and scalability. In recent years, high order discontinuous Galerkin (dG) methods have become one of the most promising tools for the solution of wave propagation problems. Indeed, thanks to their local nature, dG methods are particularly apt to treat highly heterogeneous media, complex geometries, and sharp variation of the wave field by allowing for space and time adaptivity within the approximation.

In this work, we present two different dG schemes that can be applied for the time integration of the system of second-order ordinary differential equations stemming after a dG space discretization of the wave equation. We compare the resulting discrete formulations from the point of view of stability, convergence, and computational cost, highlighting the main advantages and drawbacks of the two approaches. We present a wide set of two- and three-dimensional numerical experiments confirming the theoretical error bounds and apply the methods to realistic geophysical problems. Finally, we analyze the efficiency of the algorithm from the point of view of scalability on HPC machines.

A path conservative finite volume method for a shear shallow water model

Asha Kumari Meena

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The shear shallow water model provides an approximation for shallow water flows by including the effect of vertical shear in the model. This model can be derived from the depth averaging process by including the second order velocity fluctuations which are neglected in the classical shallow water approximation. The resulting model has a non- conservative structure which resembles the 10-moment equations from gas dynamics. This structure facilitates the development of path conservative schemes and we construct HLL, 3-wave and 5-wave HLLC-type solvers. An explicit and semi-implicit MUSCL-Hancock type second order scheme is proposed for the time integration. Several test cases including roll waves show the performance of the proposed modeling and numerical strategy.

Low-regularity integration of NLS

Alexander Ostermann

University of Innsbruck, Austria

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) Fourier 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), Katharina Schratz (Sorbonne, Paris), Yifei Wu (Tianjin University, China) *and* Fangyan Yao (South China University, Guangzhou).

Adaptive energy preserving methods for partial differential equations

Brynjulf Owren

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A framework for constructing integral preserving numerical schemes for time-dependent partial differential equations on non-uniform grids is presented. The approach can be used with both finite difference and partition of unity methods, thereby including finite element methods. The schemes are then extended to accommodate r-, hand p-adaptivity. To illustrate the ideas, the method is applied to the Korteweg–de Vries equation and the sine-Gordon equation. Results from numerical experiments are presented.

Consistent treatment of boundary conditions for viscoelastic arterial networks governed by conservative laws with relaxation terms

Francesco Piccioli

Università degli Studi di Ferrara, Italy

A noteworthy aspect of computational haemodynamics is the modelling of the mechanical interaction between blood and vessel walls. The complete viscoelastic characterisation of this latter leads to numerical results close to physiological evidence. In this work, viscoelasticity is considered in arterial networks via the Standard Linear Solid Model, allowing the introduction of a viscoelastic constitutive tube law in the governing system of equations. The implementation of the viscoelastic contribution at boundaries (inlet, outlet and internal junctions), is performed relying on the hyperbolic nature of the mathematical model. A non-linear system is formulated based on the definition of the Riemann Problem at junctions, characterised by rarefaction waves separated by contact discontinuities, among which the mass and the total energy are conserved. The numerical model consists of an asymptotic-preserving IMEX-SSP(3,3,2) Runge-Kutta Finite Volume scheme. An L-stable diagonally implicit Runge-Kutta (DIRK) scheme is chosen to treat the stiff source terms in the governing system, given by the viscoelasticity, to ensure elevated robustness. The chosen numerical model is proven to be second-order accurate in the whole domain and well-balanced, even when including junctions. Two different benchmark models of the arterial network are implemented, differing in geometry and viscoelastic parameters. The hysteresis loops in the arterial sites of the two networks highlight the high sensitivity of the model to the chosen viscoelastic parameters.

Efficient and robust step size control for computational fluid dynamics

Hendrik Ranocha

University of Hamburg, Germany

We develop error-control based time integration algorithms for compressible fluid dynamics (CFD) applications and show that they are efficient and robust in both the accuracy-limited and stability-limited regime, focusing on discontinuous spectral element semidiscretizations. We demonstrate the importance of choosing adequate controller parameters and provide a means to obtain these in practice by combining analysis with a data-driven approach, which we apply to design new controllers for existing methods and for some new embedded Runge-Kutta pairs. We compare a wide range of error-control-based methods, along with the common approach in which step size control is based on the Courant-Friedrichs-Lewy (CFL) number. The new optimized methods give improved performance and naturally adopt a step size close to the maximum stable CFL number at loose tolerances, while additionally providing control of the temporal error at tighter tolerances. The numerical examples include challenging industrial CFD applications.

Implicit-Explicit Generalized Additive Runge–Kutta Methods

Steven Roberts

Lawrence Livermore National Laboratory, USA

Historically, implicit-explicit (IMEX) Runge–Kutta methods have been represented and analyzed almost exclusively within the confines of two frameworks: Additive Runge–Kutta (ARK) and Additive Semi-Implicit Runge–Kutta (ASIRK). While numerous high-quality integrators have been developed with these frameworks, their structures have several limitations. For example, the underlying implicit and explicit methods must have the same number of stages. Order conditions and simplifying assumptions are very restrictive and tightly couple the methods together. In this presentation, we explore Generalized Additive Runge–Kutta (GARK) as a platform for constructing IMEX schemes. GARK naturally reveals hidden coupling coefficients that control the interactions between an implicit and explicit method. It encompasses ARK and ASIRK as special cases but offers roughly twice the coefficients. Using this additional flexibility, we address the aforementioned limitations and devise novel structures for IMEX methods. New methods up to order 4 suitable for ODEs and index-1 DAEs are presented and compared to existing IMEX methods.

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Linearly Implicit General Linear Methods

Adrian Sandu
Virginia Tech, USA

Linearly implicit Runge–Kutta methods provide a fitting balance of implicit treatment of stiff systems and computational cost. In this paper we extend the class of linearly implicit Runge–Kutta methods to include multi-stage and multi-step methods. We provide the order con- dition theory to achieve high stage order and overall accuracy while admitting arbitrary Jacobians. Several classes of linearly implicit general linear methods (GLMs) are discussed based on existing families such as type 2 and type 4 GLMs, two-step Runge–Kutta methods, parallel IMEX GLMs, and BDF methods. We investigate the stability implications for stiff problems and provide numerical studies for the behavior of our methods compared to linearly implicit Runge–Kutta methods. Our experiments show nominal order of convergence in test cases where Rosenbrock methods suffer from order reduction.

Implicit multi-derivative time discretization for the DG method

Jochen Schütz
UHasselt University, Belgium

In this talk, we present recent results on how to efficiently combine a discontinuous Galerkin method with a deferred correction multi-derivative time discretization. We show how to augment the spatial operator in such a way that the fully discrete scheme is stable; this ultimately results in an extended system matrix. We investigate and develop preconditioners for this extended matrix and show how to efficiently solve the resulting non-linear algebraic equations using a state-of-the-art Jacobian-free Newton-Krylov approach. Finally, numerical results for the compressible Navier-Stokes equation are shown.

Efficient and accurate structure preserving schemes for complex nonlinear systems

Jie Shen

Purdue University, USA

Many complex nonlinear systems have intrinsic structures such as energy dissipation or conservation, and/or positivity/maximum principle preserving. It is desirable, sometimes necessary, to preserve these structures in a numerical scheme. I will present some recent advances on using the scalar auxiliary variable (SAV) approach to develop highly efficient and accurate structure preserving schemes for a large class of complex nonlinear systems. These schemes can preserve energy dissipation/conservation as well as other global constraints and/or are positivity/bound preserving, only require solving decoupled linear equations with constant coefficients at each time step, and can achieve higher-order accuracy.

Fractional-Step Runge–Kutta Methods: Representation and Linear Stability Analysis

Raymond Spiteri

University of Saskatchewan, Canada

Fractional-step methods are a popular and powerful divide-and-conquer approach for the numerical solution of differential equations. When the integrators of the fractional steps are Runge–Kutta methods, such methods can be written as generalized additive Runge–Kutta (GARK) methods, and thus the representation and analysis of such methods can be done through the GARK framework. We show how the representation and linear stability of such methods are related to the individual integrators and use this framework to explain some common observations in the literature.

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