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Recent Advances in Numerics for Deterministic and Stochastic Dynamical Systems Special Session A4

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The special session is focused on presenting recent advances in numerical modeling for evolutionary problems (such as Ordinary and Partial Differential Equations, Stochastic Differential Equations). The focus of each contribution is conveyed on numerical integrators, the analysis of their relevant properties, also towards possible applications. Accuracy, stability and structure-preserving issues are considered, together with their role in selected applications. Theoretical issues are also supported by a proper selection of numerical experiments.

Schedule and Abstracts

July 23, 2024

11:00–11:45 Transient dynamics under structured perturbations: a bridge between unstructured to structured pseudospectra

Nicola Guglielmi (Gran Sasso Science Institute, ITALY)

Abstract. The structured ε-stability radius is introduced as a quantity to assess the robustness of transient bounds of solutions to linear differential equations under structured perturbations of the matrix. This applies to general linear structures such as complex or real matrices with a given sparsity pattern or with restricted range and corange, or special classes such as Toeplitz matrices. The notion conceptually combines unstructured and structured pseudospectra, allowing for the use of resolvent bounds as with unstructured pseudospectra and for structured perturbations as with structured pseudospectra, which has important applications.

We propose and study an algorithm for computing the structured ε-stability radius, which solves eigenvalue optimization problems via suitably discretized rank-1 matrix differential equations that originate from a gradient system. The proposed algorithm has essentially the same computational cost as the known rank-1 algorithms for computing unstructured and structured stability radii. Numerical experiments illustrate the behavior of the algorithm.

References

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12:00–12:45 Steady-state density preserving method for a class of second-order stochastic differential equations

Hugo de la Cruz (Fundação Getúlio Vargas, Brazil)

Abstract. We devise a method for the long-time integration of a class of damped second-order stochastic systems. The introduced numerical scheme has the advantage of being completely explicit for general nonlinear systems while, in contrast with other commonly used integrators, is able to compute the evolution of the system with high numerical stability and precision in very large time intervals. Notably, the method has the important property of preserving, for all values of the stepsize, the steady-state probability density function of any linear system

with a stationary distribution. Numerical simulations are presented to illustrate the practical performance of the introduced method.

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14:30–15:15 Nonstandard numerical integration of local and nonlocal differential models

Angelamaria Cardone (University of Salerno, Italy)

Abstract. Reliable numerical simulations of real-life applications should be based on methods able to catch the main features of the phenomenon under consideration. This means that the numerical method must preserve properties such as positivity, boundedness, monotonicity, asymptotic values, conservation laws of the exact solution.

In this talk, we focus on differential models of physical or biological phenomena, where the modelled quantities are, e.g., chemical concentrations, population sizes or the temperature, thus these should necessarily be positive. General-purpose numerical methods are not usually derived to satisfy this property, thus they may produce nonphysical solutions, at least on coarse grids. Recently, some numerical schemes have been proposed which compute positive solution by design, as the nonstandard finite difference schemes, introduced in [4].

The first part of the talk regards time-fractional reaction-advection-diffusion problems with positive solution. We apply a standard space discretization by finite difference schemes, L1 or Grünwald-Letnikov methods for the approximation of the fractional derivative in time; then we suitably modify each scheme using a nonstandard time integration, to obtain positive solutions. We analyse the stability and the convergence of the proposed schemes. We compare these methods with their standard counterpart on some significant test examples.

The second part of the talk is concerned with an age-group SIR (Susceptible-Infected-Recovered) model, which is composed by a nonlinear system of ordinary differential equations. We prove the conservation of the total population, the positivity of the analytical solution, and derive the final size of the epidemic. For the numerical approximation, we consider standard and nonstandard finite difference schemes, and a Modified Patankar-Runge-Kutta (MPRK) method. We prove that the standard finite difference scheme preserves the positivity only for a small stepsize, while the nonstandard one and the MPRK method are unconditionally positive. A model for the diffusion of information in social networks is considered for application of the presented results on real data.

References

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15:30–16:15 Stabilization of synchronous solutions in networks
Cinzia Elia (University of Bari "Aldo Moro", Italy)

Abstract. We consider a network of identical agents, coupled through linear antisymmetric nearest neighbor coupling. The single agent dynamic has an attractor and we are interested in stabilizing the corresponding synchronous solution in the network. In this talk: (i) We show how and when it is possible to choose an appropriate coupling of the agents so that the synchronous solution is stable, and (ii) we show that this guarantee of stability comes without having to let the coupling strength be too large. Our construction is based on the Master Stability Function and on solving a suitable inverse eigenvalue problem for the coupling matrix. Numerical implementations will be presented.

References

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17:00–17:45 Structure-preserving numerics: yesterday, today and tomorrow
Raffaele D'Ambrosio (University of L'Aquila, Italy)

Abstract. This talk aims to outline some recent advances on structure-preserving numerical methods for deterministic and stochastic differential equations, highlighting the basic principles of the so-called geometric numerical integration by its history. After providing a glance to deterministic structure-preservation, the talk moves towards the direction of stochastic geometric numerical integration, according to the following two directions:

- *track 1: geometric numerical integration of stochastic Hamiltonian problems.* For these problems, two different scenarios are visible: 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 case, 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 under the exact dynamics. Our goal is to analyze whether they can also be reproduced 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 talk also aims to address tentative future directions for geometric numerical integration and a vision of potentially new fields of inspection where structure preservation can be directly involved.

References

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July 24, 2024

11:30–12:15 Derivation of new linearly implicit methods for stiff PDEs models
Dajana Conte (University of Salerno, Italy)

Abstract. Partial Differential Equations (PDEs) constitute one of the most common tools for modeling several phenomena. This talk focuses on the efficient numerical solution of PDEs models coming from real applications, such as corrosion of materials, sustainability (Maldon et al., Entropy, 2020), vegetation (Eigentler et al., Bull. Math. Biol., 2019). The numerical treatment of these models is not trivial, since a related spatial discretization, performed e.g. via finite differences, finite elements, spectral methods, often leads to large and highly stiff Initial Value Problems (IVPs). These two issues are difficult to treat simultaneously: in fact, the stiffness could force the use of very dense temporal grids, which however would make the computational cost of the method very high, due to the non-negligible size of the problem.

In this talk, we propose new efficient linearly implicit numerical methods for solving large and highly stiff problems. They are derived by stabilizing explicit numerical schemes through the so-called TASE (Time-Accurate and highly-Stable Explicit) preconditioners [1].

In particular, to improve the classical TASE-RK methods [2], starting from them we derive two new classes of numerical schemes: TASE-peer methods [3], which can be parallelized; AMF TASE-W methods [5], which have better stability properties than TASE-RK, and require the solution of a lower number of linear systems per integration step.

We finally show the derivation of adapted discretizations for two reaction-diffusion PDEs models: one for the corrosion of metallic materials [6], and one for vegetation growth in the African Savannah [4]. Numerical results testify the efficiency of the proposed methods.

References

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12:30–12:50 A spectral method for dispersive solutions of the nonlocal Sine-Gordon equation
Sabrina Francesca Pellegrino (Polytechnic University of Bari, Italy)

Abstract. Moved by the pressing need for rigorous and reliable numerical tools for the analysis of peridynamic materials, the authors propose a model able to capture the dispersive features of nonlocal soliton-like solutions obtained by a peridynamic formulation of the Sine-Gordon equation. The analysis of the Cauchy problem associated to the peridynamic Sine-Gordon equation with local Neumann boundary condition is performed in this work through a spectral method on Chebyshev polynomials nodes joined with the Störmer-Verlet scheme for the time evolution. The choice for using the spectral method resides in the resulting reachable numerical accuracy, while, indeed, Chebyshev polynomials allow straightforward implementation of local boundary

conditions. Several numerical experiments are proposed for thoroughly describe the ability of such scheme. Specifically, dispersive effects as well as the ability of preserving the internal energy of the specific peridynamic kernel are demonstrated.

References

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14:30–15:15 Optimization of eigenvalues based on dynamical low-rank
Carmela Scalone (University of L'Aquila, Italy)

Abstract. The use of techniques based on dynamical low-rank approximation in eigenvalue problems, when the underlying solution has a low-rank structure, has proven to be very effective, both in the case of the rightmost eigenpairs of linear operators and in the computation of the effective eigenvalue for the neutron transport equation. In this talk, we focus on the latter problem. In particular, we consider a previously introduced special low-rank inverse power iteration, which is very efficient in lowering memory requirements, and provide suitable rank adaptations. We focus on a combination of the aforementioned method with techniques to optimise quantities of interest in order to obtain specific values of the effective eigenvalue. This is a joint work with L. Einkemmer, J. Kusch and R. McClarren.

References

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15:30–16:15 An IVP solver for Filippov systems on co-dimension 2 manifolds and regularizations for the moments vector field
Fabio Vito Difonzo (Istituto per le Applicazioni del Calcolo "Mauro Picone", Consiglio Nazionale delle Ricerche, Italy)

Abstract. We present a numerical solver for the integration of systems with discontinuous right-hand side, enabling sliding dynamics on co-dimensional 1 manifolds and 2. It is based on an adaptive Runge Kutta-type integrator, coupled with event detection for switch between different regimes, and on the method of moments to define the slip. The latter method can automatically detect co-dimensional 2 tangential exits. We further monitor other general exit points that may occur. Indeed, a co-dimension 2 discontinuity manifold can be attractive in finite time by partial sliding or spiraling.

Moreover, we introduce a novel regularization for discontinuous vector fields that is able to overcome issues of the bilinear regularization near first order tangential exit points and that is conjectured to converge to the moments vector field on the discontinuity manifold.

17:00–17:20 Numerical preservation of stochastic dissipativity
Helena Biscevic (Gran Sasso Science Institute, Italy)

Abstract. 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 some future frontiers concerning numerical dissipativity for stochastic partial differential equations.

References

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17:30–18:15 Adaptive Tau-Leaping Strategies for Efficient Kinetic Monte Carlo Simulations in Spatially Non-Uniform Systems

Xiaoying Han (Auburn University, USA)

Abstract. In this presentation, we address the computational challenges encountered by traditional Kinetic Monte Carlo (KMC) approaches, particularly in systems with diverse timescales and spatial non-uniformity. Our work focuses on enhancing the efficiency of KMC time integration, with a specific emphasis on lattice structures in surface chemistry applications. We introduce two novel adaptive tau-leaping methods and their associated time integration strategies, inspired by the "n-fold" direct KMC approach. These methods enable simultaneous execution of multiple reactions, advancing time using adaptively-selected coarse increments, thereby significantly improving computational efficiency. Through numerical experiments, we demonstrate the efficacy of our proposed methods in comparison to existing approaches, using a catalytic surface kinetics application involving ammonia decomposition as a case study. Our findings underscore the promising potential of these strategies to streamline KMC simulations in spatially heterogeneous kinetic systems, paving the way for broader applications in complex reaction environments.

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