Sesión Especial 13

Advanced methods for differential problems and their applications

Organizers:

- Severiano González-Pinto (University of La Laguna)
- Inmaculada Higueras (Public University of Navarre)
- Juan Ignacio Montijano (University of Zaragoza)

Summary:
The aim of this Mini-Symposium is to promote, encourage, cooperate, and bring together researchers in the fields of the numerical solution of differential problems and their applications. In particular, special attention will be dedicated to the time-integration through the analysis, construction and development of efficient numerical methods which are able to accurately preserve the qualitative and quantitative behavior of the theoretical solution. Applications in different contexts will also be considered.

Program

THURSDAY, 25th of January:

11:30 – 12:00	Marnix Van Daele (Ghent University) *A new method to solve the 2D Schrödinger equation*
12:00 – 12:30	Dajana Conte (University of Salerno) *Taylored numerical modeling of reaction-diffusion PDEs from applications*
12:30 – 13:00	Raffaele D'Ambrosio (Universita degli studi dell' Aquila) *Numerical preservation principles for stochastic dynamical systems*
13:00 – 13:30	Domingo Hernández-Abreu (University of La Laguna) *AMF-TASE-W methods for the time integration of parabolic PDEs*
16:00 – 16:30	Teo Roldán (Public University of Navarre) *Reduction of the computational cost of aeroelastic codes for wind turbine*
16:30 – 17:00	Juan Ignacio Montijano (University of Zaragoza) *W-methods with reduced evaluations of the vector field*
17:00 – 17:30	Luis Rández (University of Zaragoza) *Three-stage Peer methods for the numerical solution of second order IVPs*
17:30 – 18:00	Inmaculada Higueras (Public University of Navarre) *Strong stability for Runge–Kutta schemes on a class of nonlinear problems revisited*

A new method to solve the 2D Schrödinger equation

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Abstract: We consider the numerical solution of the two-dimensional linear time-independent Schrödinger equation

$$-\nabla^2\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y)\,,$$

on a bounded, sufficiently regular domain $\Omega \subset \mathbb{R}^2$ subject to homogeneous Dirichlet boundary conditions. The solutions consist of real eigenvalues E and corresponding eigenfunctions $\psi(x,y)$.

The method we propose here is inspired by Ixaru, who presented in [1] an adaptation of a well-known technique developed by Titchmarsch: in the x-direction the eigenfunction is expressed in well-chosen, yet y-dependent sets of basis functions. Another inspiring idea was found in [2], where the authors propose a simple, easy to implement method based upon high order finite difference approximations. Numerical examples were reported with similar accuracies as the method in [1].

The combination of these two ideas, together with the improvements from [3] and the use of very efficient algorithms for solving the one-dimensional Schrödinger equations [4], leads to a new method.

References

[1] L. Gr. Ixaru (2010). New numerical method for the eigenvalue problem of the 2D Schrödinger equation. Comput. Phys. Commun., 181, 1738–1742.

[2] Z. Wang and H. Shao (2009). A new kind of discretization scheme for solving a two-dimensional time-independent Schrödinger equation. Comput. Phys. Commun., 180, 842-849.

[3] T. Baeyens and M. Van Daele (2022). Improvements to the computation of eigenvalues and eigenfunctions of two-dimensional Schrödinger equations by constant perturbation based algorithms. J. Comput. Appl. Math., 412, 114292.

[4] T. Baeyens and M. Van Daele (2021). The fast and accurate computation of eigenvalues and eigenfunctions of time-independent one-dimensional Schröödinger equations. Comput. Phys. Commun., 258, 107568.

Taylored numerical modeling of reaction-diffusion PDEs from applications

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Abstract: We consider the numerical solution of reaction-diffusion models from applications, among which we mention: corrosion of metallic materials [2] (Mai et al. 2016, Waschinsky et al. 2021); deterioration of architectural works [1]; vegetation phenomena [4] (Eigentler et al. 2019). These models are often characterized by high stiffness and a-priori known properties, such as conservation laws, positivity, oscillating and long-term behavior of the solution, which would be appropriate to preserve in the discrete setting for choices of large step-sizes [2, 3, 4].
To this end, we propose new problem-taylored numerical methods, based on the improvement and/or generalization of known techniques, such as exponential fitting, non-standard finite differences, TASE preconditioners [5] (Calvo et al. 2021). Numerical results testify that the shown methods are competitive in solving reaction-diffusion models from applications.

References

[1] F. Colace, D. Conte, G. Frasca-Caccia, A. Lorusso, D. Santaniello, C. Valentino (2023). An IoT-based framework for the enjoyment and protection of Cultural Heritage Artifacts. TwinNets.

[2] D. Conte, G. Frasca-Caccia (2022). A MATLAB code for the computational solution of a phase field model for pitting corrosion. Dolomites Res. Notes Approx., 15(2), 47–65.

[3] D. Conte, G. Frasca-Caccia (2023). Exponentially fitted methods with a local energy conservation law. Adv. Comput. Math., 49(4), 49.

[4] D. Conte, G. Pagano, B. Paternoster (2023). Nonstandard finite differences numerical methods for a vegetation reaction-diffusion model. J. Comput. Appl. Math., 419, 114790.

[5] D. Conte, G. Pagano, B. Paternoster (2023). Time-accurate and highly-stable explicit peer methods for stiff differential problems. Commun. Nonlinear Sci. Numer. Simul., 119, 107136.

Numerical preservation principles for stochastic dynamical systems

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Abstract: The talk is aimed to highlight some principles of stochastic geometric numerical integration, i.e., on the ability of numerical methods to preserve characteristic features of stochastic dynamics. In particular, the attention is focused on stochastic differential equations satisfying some characteristic invariance laws. The behaviour of stochastic one-step methods in the preservation of mean-square contractivity will be analyzed. The analysis will also be conveyed to the discretization of stochastic Hamiltonian problems and the numerical long-term preservation of the behavior of the expected Hamiltonian. The theoretical analysis will also be supported by selected numerical tests.

AMF-TASE-W methods for the time integration of parabolic PDEs

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Abstract: We consider the application of the Approximate Matrix Factorization in combination with TASE W-methods [1, 2, 4] for the numerical solution of semi-discrete parabolic Partial Differential Equations. Although for AMF W-methods the temporal order of consistency is immediately obtained from that of the underlying W-method, such property needs further discussion for the newly introduced AMF-TASE W-methods. It is shown [3] that the parallel structure of the latter methods allows to retain the order of consistency of the underlying TASE W-method. Numerical experiments will be presented to assess the consistency result and to show that the proposed schemes are competitive to existing AMF W-methods.

Joint work with Severiano González-Pinto (University of La Laguna) and Dajana Conte and Giovanni Pagano (University of Salerno).

References

[1] M. Bassenne, L. Fu and A. Mani (2021). Time-Accurate and highly-Stable Explicit operators for stiff differential equations. J. Comp. Phys., 424, 109847.

[2] M. Calvo, J.I. Montijano and L. Rández (2021). A note on the stability of time-accurate and highly-stable explicit operators for stiff differential equations. J. Comp. Phys., 436, 110316.

[3] D. Conte, S. González-Pinto, D. Hernández-Abreu and G. Pagano (2023). On Approximate Matrix Factorization and TASE W-methods for the time integration of parabolic Partial Differential Equations. Submitted for publication.

[4] S. González-Pinto, D. Hernández-Abreu, G. Pagano and S. Pérez-Rodríguez (2023). Generalized TASE-RK methods for stiff problems. Appl. Numer. Math., 188, 129-145.

Reduction of the computational cost of aeroelastic codes for wind turbines

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Abstract: In recent wind turbine designs, larger and more powerful machines are increasingly used with the aim of reducing installation and maintenance costs. This increase in rotor size and blade flexibility requires, for a more realistic representation of the physics of the new designs, the development of higher-level models. Consequently, the computational cost required to perform the calculations increases.
The main objective of this study is to reduce the computational cost of some advanced modelling codes.This will enable improved machine design, evaluation and certification processes in industry.
Much of the computational cost in numerical simulation codes is due to spatial discretization and temporal integration of the differential problem associated with the model. A small number of numerical methods (RK4, PCC, PC2B,...) are currently used in the wind turbine literature. However, in the field of numerical simulation there are a variety of schemes, some of which could work very well in this context, such as IMEX methods, RK methods specific to stiff problems, variable step implementation, error estimation, other spatial discretizations.
Joint work with Inmaculada Higueras (Public University of Navarre), and Raquel Martín San Román (National Renewable Energy Centre (CENER).

References

[1] K. M. Kecskemety, J. J. McNamara (2011). Influence of wake effects and inflow turbulence on wind turbine loads. AIAA Journal, 49(11), 2564–2576.

[2] J. G. Leishman, M. J. B., and A. Bagai (2002). Free-vortex filament methods for the analysis of helicopter rotor wakes. Journal of Aircraft, 39(5), 759–775.

[3] R. Martín-San-Román, P. Benito-Cia, J. Azcona-Armendáriz, A. Cuerva-Tejero (2021). Validation of a free vortex filament wake module for the integrated simulation of multi-rotor wind turbines. Renewable Energy179, 1706–1718.

W-methods with reduced evaluations of the vector field

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Abstract: In this talk, we present a new family of W-methods for the numerical solution of stiff initial value problems. These methods have a special structure in which some of the evaluations of the vector field are re-used in one or several stages, reducing in this way its computational cost. This can be very convenient when the evaluation of the derivative function is expensive. The properties of accuracy and stability are studied. Some numerical experiments show the performance of the new methods.
Joint work with Severiano González-Pinto and Domingo Hernández-Abreu (University of La Laguna), and Luis Rández (Universidad de Zaragoza).

References

[1] S. González-Pinto, D. Hernández-Abreu, G. Pagano, S. Pérez-Rodríguez. Generalized TASE-RK methods for stiff problems. To appear in Appl. Numer. Math.

[2] T. Steihaug and A. Wolfbrandt (1979). An attempt to avoid exact Jacobian and nonlinear equations in the numerical solution of stiff differential equations. Math. Comp. 33, No. 146, 521–534.

Three-stage Peer methods for the numerical solution of second order IVPs

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Abstract: In this work, we solve numerically second order initial vale problems $y'' = f(t,y)$ by means of 3-stage explicit two-step Peer methods, given by

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

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

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

We propose a 3-stage method with one reused stage, so that only two effective function evaluations of the derivative are needed per step. We analyze the 0-stability, consistency and convergence of a particular scheme of order five.

References

[1] S. Jebens, R. Weiner, H. Podhaisky, B.A. Schmitt (2008). Explicit multi-step peer methods for special second-order differential equations. Applied Mathematics and Computation, 202, 803–813.

Strong stability for Runge–Kutta schemes on a class of nonlinear problems revisited

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Abstract: We consider the numerical preservation of qualitative properties (monotonicity, contractivity, positivity, etc.) when explicit Runge–Kutta (RK) methods are used to solve a class of nonlinear differential problems. This issue was studied in [1] in the framework of Strong Stability Preserving (SSP) methods, and new modified threshold factors were defined. For many methods, the stepsize restrictions obtained with this approach were better than the ones given in terms of the Kraaijevanger's coefficient in the SSP theory. However, some open questions were posed in [1]. In this talk we go deeper in this topic. Some numerical experiments are given to illustrate the results obtained.

References

[1] I. Higueras, (2013). Strong stability for Runge–Kutta schemes on a class of nonlinear problems. J. Sci. Comput., 57, 518-535.