Sesión Especial 16

Integración temporal de ecuaciones diferenciales

Organizadores

- Severiano González-Pinto (Universidad de La Laguna)
- Inmaculada Higueras (Universidad Pública de Navarra)
- Juan Ignacio Montijano (Universidad de Zaragoza)

Descripción

El objetivo de la sesión especial es mostrar los últimos avances en métodos numéricos para la integración temporal de ODEs y PDEs en el contexto del método de líneas.

Programa

Martes, 5 de febrero (mañana)

11:30 – 12:00	Ernst Hairer (Université de Genève) *Long-time behaviour of numerical integrators for charged particle dynamics*
12:00 – 12:30	Luigi Brugnano (Universitá degli Studi di Firenze) *Spectral Hamiltonian Boundary Value Methods (SHBVMs)*
12:30 – 13:00	Pep Mulet Mestre (Universitat de València) *Implicit-explicit schemes for partial differential equations with a nonlocal gradient flow structure*
13:00 – 13:30	Laura Portero (Universidad Pública de Navarra) *Parallel space-time algorithms for the solution of parabolic problems*

Martes, 5 de febrero (tarde)

17:00 – 17:30	Inmaculada Higueras (Universidad Pública de Navarra) *Optimal monotonicity–preserving perturbations of a given Runge-Kutta method*
17:30 – 18:00	Domingo Hernández Abreu (Universidad de La Laguna) *On step-size control for Radau IIA methods by means of two-step error estimators*
18:00 – 18:30	Teo Roldán (Universidad Pública de Navarra) *On Low-Storage SSP(5,3) Runge-Kutta methods*
18:30 – 19:00	Luis Rández (Universidad de Zaragoza) *L-stable singly implicit Peer methods for the solution of stiff IVPs*

Long-time behaviour of numerical integrators for charged particle dynamics

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Abstract. The Boris algorithm is the most popular time integrator for charged particle motion in electric and magnetic force fields. It is a symmetric one-step method, and it preserves the phase volume exactly. However, it is not symplectic.
In this talk we prove near-conservation of energy over very long times in the special cases where either the magnetic field is constant or the electric potential is quadratic. When none of these assumptions is satisfied, it is illustrated by numerical examples that the numerical energy can have a linear drift or its error can behave like a random walk.
We thank Martin Gander for drawing our attention to this problem.

References

[1] E. Hairer and C. Lubich, *Energy behaviour of the Boris method for charged-particle dynamics*, BIT, to appear.

[2] E. Hairer and C. Lubich, *Long-term analysis of a variational integrator for charged-particle dynamics in a strong magnetic field*, Submitted for publication.

This talk is based on joint-work with Christian Lubich.
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Spectral Hamiltonian Boundary Value Methods (SHBVMs)

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Abstract. *Hamiltonian Boundary Value Methods (HBVMs)* [1] can be regarded as spectral methods in time along the orthonormal Legendre basis. Their usage in such a fashion has begun only recently, by using the methods for solving highly-oscillatory problems [4] and stiffly-oscillatory problems [2], which has led to define *Spectral HBVMs (SHBVMs)*. This has been possible because of the very efficient nonlinear iteration available for solving the generated discrete problems [3]. In this talk, we report the main facts concerning this approach, as well as recent findings in SHBVMs.

References

[1] L. Brugnano, F. Iavernaro, *Line Integral Methods for Conservative Problems.* Chapman and Hall/CRC, Boca Raton, FL, 2016.

[2] L. Brugnano, F. Iavernaro, J.I. Montijano, L. Rández, *Spectrally accurate space-time solution of Hamiltonian PDEs.* (2018) `https://doi.org/10.1007/s11075-018-0586-z`

[3] L. Brugnano, F. Iavernaro, D. Trigiante, *A note on the efficient implementation of Hamiltonian BVMs.* J. Comput. Appl. Math. **236** (2011) 375–383.

[4] L. Brugnano, J.I. Montijano, L. Rández, *On the effectiveness of spectral methods for the numerical solution of multi-frequency highly-oscillatory Hamiltonian problems.* Numer. Algorithms (2018) `http://dx.doi.org/10.1007/s11075-018-0552-9`

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Implicit-explicit schemes for partial differential equations with a nonlocal gradient flow structure

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Abstract. The work in [1] is concerned with numerical methods for a nonlinear nonlocal equations with a gradient flow structure that arises in models for collective behavior. The numerical solution of this problem by an explicit finite difference method is costly due to the spatial convolution in the convective numerical flux, and due to the disadvantageous CFL condition incurred by the diffusion term. Based on explicit schemes for such models devised in [2] a second-order implicit-explicit Runge-Kutta (IMEX-RK) method can be formulated. This method avoids the restrictive time step limitation of explicit schemes since the diffusion term is handled implicitly. Although this entails solving nonlinear algebraic systems in every time step, numerical experiments illustrate the relative efficiency of this proposal.

References

[1] R. Bürger, D. Inzunza, P. Mulet, *Implicit-explicit schemes for nonlinear nonlocal equations with a gradient flow structure in one space dimension*, to appear in Numerical Methods in PDE, 2018.

[2] J.A. Carrillo, A. Chertock, Y. Huang, *A finite-volume method for nonlinear nonlocal equations with a gradient flow structure*, Commun. Comput. Phys. vol. 17 (2015) pp. 233–258.

Joint work with Raimund Bürger, Daniel Inzunza (U. Concepción, Chile) y Luis Miguel Villada (U. Bio Bio, Chile).
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Parallel space-time algorithms for the solution of parabolic problems

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Abstract. Classical domain decomposition techniques provide efficient numerical strategies for the parallel solution of elliptic problems. Nevertheless, the use of such techniques in the context of parabolic problems encounters a bottleneck due to sequential time integration procedures. Since the development of new computer architectures is moving towards increasing the number of cores rather than improving their clock speed-up, it is convenient to look for numerical methods that allow for time parallelization. In this framework, this work proposes and analyzes the combination of domain decomposition splitting time integrators with parallel-in-time techniques such as parareal and waveform relaxation methods (cf. [1, 2, 3] and references therein).

References

[1] M.J. Gander, *50 years of time parallel time integration*, *Multiple shooting and time domain decomposition methods*, Contrib. Math. Comput. Sci. 9, pp. 69–113, Springer, Cham, 2015.

[2] M.J. Gander and S. Vandewalle, *Analysis of the parareal time-parallel time-integration method*, SIAM J. Sci. Comput. 29, (2007), 556–578.

[3] S. Vandewalle, *Parallel multigrid waveform relaxation for parabolic problems*, Teubner Skr. Numer., B.G. Teubner, Stuttgart, 1993.

Joint work with Andrés Arrarás, Francisco J. Gaspar and Carmen Rodrigo.
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Optimal monotonicity–preserving perturbations of a given Runge-Kutta method

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Abstract. Perturbed Runge–Kutta methods (also referred to as downwind RK methods) can guarantee monotonicity preservation under larger step sizes relative to their traditional Runge–Kutta counterparts. In this talk we we show how to optimally perturb a given method in order to increase the radius of a.m. We prove that for methods with zero radius of a.m., it is always possible to give a perturbation with positive radius. We first study methods for linear problems and then methods for nonlinear problems. In each case, we prove upper bounds on the radius of a.m. and provide algorithms to compute optimal perturbations. Optimal perturbations for many known methods are given. The numerical experiments done prove the sharpness of the new step size restrictions [1].

References

[1] I. Higueras, D. Ketcheson, and T.A. Kocsis, *Optimal monotonicity–preserving perturbations of a given Runge-Kutta method*. J. Sci. Comput, 76 (3):1337–1369, 2018.

Joint work with D. Ketcheson and T. A. Kocsis.
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On step-size control for Radau IIA methods by means of two-step error estimators

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Abstract. We shall discuss error estimators for $s-$stage RadauIIA methods based on two consecutive steps through embedded methods of the form

$$\hat{y}_{n+1} = y_n + h_{n-1}\sum_{i=1}^{s}\hat{d}_{n,i}f(Y_{n-1,i}) + h_n\sum_{i=1}^{s}\hat{b}_{n,i}f(Y_{n,i}),$$

where $\{Y_{n-j,i}\}_{i=1}^{s}$ are the internal stages computed at time t_{n-j}, $j = 0, 1$, and $\{\hat{d}_{n,i}, \hat{b}_{n,i}\}_{i=1}^{s}$ are certain coefficients to be conveniently selected. Embedded methods of order s with damping for the stiff components regardless of the step-size ratio h_n/h_{n-1} are provided for $2 \le s \le 7$. Numerical experiments will be presented to illustrate the performance of the newly proposed error estimator for the case $s = 3$ incorporated in the RADAU5 code.
The authors are very grateful to Professor Ernst Hairer for his consent to use and modify the code RADAU5..

References

[1] S. González-Pinto, J.I. Montijano, S. Pérez-Rodríguez, *Two-Step Error Estimators For Implicit Runge-Kutta Methods Applied to Stiff Systems*, ACM Trans. Math. Soft., 30 no.1 (2004) 1-18.

[2] E. Hairer, G.Wanner, *Solving Ordinary Differential Equations II, Stiff and Differential Algebraic Problems*, Springer 2^{nd} ed., Berlin, 1996.

Joint work with S. González-Pinto and J.I. Montijano.
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On Low-Storage SSP(5,3) Runge-Kutta methods

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Abstract. Time stepping Strong Stability Preserving (SSP) methods preserve, under certain step size restrictions, strong stability properties of the numerical solution. On the other hand, for high dimension ODEs, the computer memory capacity may be compromised and low memory usage strategies must be incorporated. In the context of SSP explicit Runge–Kutta schemes, some low-storage methods have been considered in the literature.

In this talk we study the family of third order 5-stage SSP explicit Runge–Kutta methods (SSP(5,3)). First, we analyze some properties of the optimal schemes, obtaining the *best* optimal SSP(5,3) methods. However, as any of them can be implemented in $2N$ memory registers, the study is extended to non-optimal SSP(5,3) methods. In this way, we achieve $2N$ low-storage SSP(5,3) schemes with SSP coefficients close to the optimal one and some other relevant properties. [1]

References

[1] I. Higueras and T. Roldán, *New third order low-storage SSP explicit Runge-Kutta methods*, 2018; arXiv:1809.04807.

Joint work with I. Higueras

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L-stable singly implicit Peer methods for the solution of stiff IVPs

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Abstract. In this paper a one parameter family of s-stage singly implicit two-step peer (SIP) methods with order $(s-1)$ that are L-stable has been developed. General peer methods are multistage two-step methods for solving IVPs where all stages possess essentially the same accuracy and stability properties. In particular a s-stage SIP requires at each step the solution of s-implicit non-linear systems of equations of the same type in a similar way to the singly implicit Runge-Kutta methods. Here for each $(s \geq 3)$ a family of one parameter s-stage SIP methods with order $(s-1)$ is derived. For $s \leq 8$ intervals of values of the parameter that ensure L-stability are obtained. Further it is shown that under some restriction on the parameter each s-stage SIP method can be formulated as a cyclic multistep method of order $(s-1)$ and this implies that the Dahlquist barrier of second-order for A-stable linear multistep methods can be broken with suitable s-stage cyclic methods of these families.

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