Total Variation Diminishing Implicit Runge–Kutta Methods for Dissipative Advection–Diffusion Problems in Astrophysics

Natalie Happenhofer[1,*], **Othmar Koch**[1,**], **Friedrich Kupka**[1,***], and **Florian Zaussinger**[2]

[1] University of Vienna, Faculty of Mathematics, Nordbergstrasse 15, A-1090 Wien, Austria

[2] Brandenburg University of Technology Cottbus, Department of Aerodynamics and Fluid Mechanics, D-03046 Cottbus , Germany.

We investigate the properties of dissipative full discretizations for the equations of motion associated with models of flow and radiative transport inside stars. We derive dissipative space discretizations and demonstrate that together with specially adapted *total-variation-diminishing (TVD)* or *strongly stable* Runge–Kutta time discretizations with adaptive step-size control this yields reliable and efficient integrators for the underlying high-dimensional nonlinear evolution equations. For the most general problem class, fully implicit SDIRK methods are demonstrated to be competitive when compared to popular explicit Runge–Kutta schemes as the additional effort for the solution of the associated nonlinear equations is compensated by the larger step-sizes admissible for strong stability and dissipativity. For the parameter regime associated with semiconvection we can use partitioned IMEX Runge-Kutta schemes, where the solution of the implicit part can be reduced to the solution of an elliptic problem. This yields a significant gain in performance as compared to either fully implicit or explicit time integrators.

1 The ANTARES Code

In this paper we discuss the numerical properties of implicit *total–variation–diminishing (TVD)* Runge–Kutta methods for simulations of stellar convection and diffusion. The ultimate goal of this investigation is to improve the computational efficiency of simulations in highly challenging parameter regimes which arise for example in A-type stars by breaking the limits imposed on the time step-sizes by the TVD requirement for classical explicit time integrators. The fundamental equation of motion is the *fully compressible Navier–Stokes equation* which describes momentum conservation. The model is completed by a *continuity equation* which ensures conservation of mass, and a *total energy equation* which describes conservation of the latter. The equations incorporate a radiative source term Q_{rad} which is determined as the stationary limit of the *radiative transfer equation*. The equations of hydrodynamics are closed by the equation of state which describes the relation between the thermodynamic quantities. For the initial condition, a slightly perturbed static model atmosphere or envelope is used which is equipped with a small seed velocity field or density perturbation to start dynamics away from equilibrium. Boundary conditions are based on the assumption that all quantities are periodic in both horizontal directions. For the hydrodynamical equations, *closed* (Dirichlet) boundary conditions at the upper and lower boundary of the computational domain are used, but a recent development is to replace these by *open* (Robin) boundary conditions. For the radiative transfer equation, incoming radiation at the boundary of the computational domain must be specified. For details of the model see [1, 2].

The ANTARES code (**A N**umerical **T**ool for **A**strophysical **RES**earch [1]) we discuss here solves this system of equations numerically in either one, two, or three spatial dimensions on a rectangular grid. ANTARES allows the definition of several grids which can be nested inside each other to improve resolution in regions of interest. The code is fully scalable on parallel architectures with MPI and OpenMP directives.

For the spatial discretization of the hyperbolic terms, discretizations of ENO (*essentially non-oscillatory*) type [3, 4] are implemented. These methods use adaptive stencils which are chosen such as to avoid spurious oscillations in the computed solution. The spatial derivatives are calculated for each direction separately.

The parabolic terms are discretized by dissipative finite difference schemes of fourth order. The *radiative heating rate* is determined by the *short characteristics method*, or by means of a diffusion approximation, where appropriate, while all other source terms are evaluated at the cell centers. For the time integration, *total variation diminishing* Runge–Kutta methods are employed. In this work we put forward fully implicit *singly diagonally implicit (SDIRK)* Runge–Kutta methods ([5] and references therein) and *implicit–explicit (IMEX)* partitioned Runge–Kutta methods ([6–8] and references therein) to replace the classical explicit integrators [9, 10].

2   Comparisons of TVD Runge–Kutta Methods

In an abstract setting, we now discuss the numerical solution of the (autonomous) initial value problem $y'(t) = F(y(t))$, $y(0) = y_0$ by an implicit s-stage Runge–Kutta method.

Ferracina & Spijker [5] introduce two classes of s-stage *Singly Diagonally Implicit Runge–Kutta (SDIRK)* methods with the TVD property of convergence orders $p = 2$ and $p = 3$, respectively. The CFL numbers, which represent a step-size restriction ensuring the TVD property, for these schemes were proven to be equal to $2s$ for each $s \geq 1$ for the second order case and $s - 1 + \sqrt{s^2 - 1}$ for the third order methods.

For the parameter regime associated with the *semiconvection problem* [11], the equations of motion can be recast as a partitioned problem $\dot{y}(t) = F(y(t)) + G(y(t))$, $y(0) = y_0$, which suggests to apply partitioned implicit–explicit Runge–Kutta methods. [6–8] put forward and analyse the TVD property for several schemes of this type.

The methods introduced above are analyzed with respect to their linear stability and *dissipativity* [12], which characterizes the step-sizes which ensure a damping of highly oscillatory modes for a given spatial discretization. We compare the left boundaries of the stability regions, the points where the *amplification factor g* characterizing dissipativity might start oscillating ($g = 0$, where an asterisk indicates a zero with a sign change) or even amplifies oscillations ($|g| = 1$) for a dissipative fourth-order space discretization put forward and analyzed in [13], and additionally the error constants C. The methods we compare are three IMEX methods characterized by parameters 'SSP$k(s, \sigma, p)$' [6], the forward Euler method, two classical explicit integrators [9, 10] and the fully implicit SDIRK methods [5]. It turns out that the largest time steps are admissible for the SDIRK methods, which however has to be contrasted with the additional effort for the solution of the associated nonlinear equations. For the IMEX methods, the nonlinear equations can be reduced to the solution of generalized Poisson equations which implies some moderate computational effort. The classical explicit integrators cannot be recommended based on this analysis.

Method	Stability	$g = 0$	$|g| = 1$	C
IMEX SSP2$(2, 2, 2)$	$-\infty$	0.452*	—	5.17
IMEX SSP2$(3, 3, 2)$	$-\infty$	0.455*	—	8.05
IMEX SSP3$(3, 3, 3)$	-3.248	0.348*	0.609	11.6
Forward Euler	-2	0.187*	0.375	12.6
Osher/Shu 2	-2	—	0.375	16.2
Osher/Shu 3	-2.512	0.299*	0.471	22.8
SDIRK $p = 2$, $s = 2$	$-\infty$	0.75	—	1.64
SDIRK $p = 2$, $s = 3$	$-\infty$	1.125*	—	0.72
SDIRK $p = 2$, $s = 4$	$-\infty$	1.5	—	0.40
SDIRK $p = 3$, $s = 2$	-12.93	—	2.424	1.43
SDIRK $p = 3$, $s = 3$	-37.10	1.746*	6.955	0.56
SDIRK $p = 3$, $s = 4$	-60.98	—	11.44	0.30

Table 1   Summary of the analysis of TVD integrators.

References

[1] H. Muthsam, F. Kupka, B. Löw-Baselli, C. Obertscheider, M. Langer, and P. Lenz, New Astronomy **15**, 460–475 (2010).
[2] A. Weiss, W. Hillebrandt, H. Thomas, and H. Ritter, Cox and Giuli's Principles of Stellar Structure, 2nd edition, Advances in Astronomy and Astrophysics (Cambridge Scientific Publishers Ltd., Cambridge, U.K., 2004).
[3] C. W. Shu, Essentially non-oscillarory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws, Tech. Rep. ICASE 97-65, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, VA, 1997.
[4] X. Liu and S. Osher, J. Comput. Phys. **142**, 304–330 (1998).
[5] L. Ferracina and M. Spijker, Appl. Numer. Math. **58**, 1675–1686 (2008).
[6] L. Pareschi and G. Russo, J. Sci. Comput. **25**, 129–155 (2005).
[7] I. Higueras, SIAM J. Numer. Anal. **44**, 1735–1758 (2006).
[8] I. Higueras, J. Sci. Comput. **39**, 115–128 (2009).
[9] C. W. Shu, SIAM J. Sci. Statist. Comput. **9**, 1073–1084 (1988).
[10] C. W. Shu and S. Osher, J. Comput. Phys. **77**, 439–471 (1988).
[11] F. Zaussinger and H. Spruit, Semiconvection, Submitted to Astronomy and Astrophysics, 2011.
[12] J. Strikwerda, Finite Difference Schemes and Partial Differential Equations, 2nd edition (SIAM, Philadelphia, PA, 2004).
[13] O. Koch, F. Kupka, B. Löw-Baselli, A. Mayrhofer, and F. Zaussinger, SDIRK methods for the ANTARES code, ASC Report 32/2010, Inst. for Anal. and Sci. Comput., Vienna Univ. of Technology, 2010, available at http://www.asc.tuwien.ac.at/preprint/2010/asc32x2010.pdf.