Received: 7 June 2021 | Accepted: 24 August 2021

DOI: 10.1002/pamm.202100027

Recent Developments in the Field of Modified Patankar-Runge-Kutta-methods

Thomas Izgin[1,*], **Stefan Kopecz**[1,**], and **Andreas Meister**[1,***]

[1] Institute of Mathematics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Modified Patankar-Runge-Kutta (MPRK) schemes are numerical one-step methods for the solution of positive and conservative production-destruction systems (PDS). They adapt explicit Runge-Kutta schemes in a way to ensure positivity and conservation of the numerical approximation irrespective of the chosen time step size. Due to nonlinear relationships between the next and current iterate, the stability analysis for such schemes is lacking. In this work, we introduce a strategy to analyze the MPRK22(α)-schemes in the case of positive and conservative PDS. Thereby, we point out that a usual stability analysis based on Dahlquist's equation is not possible in order to understand the properties of this class of schemes.

1 Introduction

Many applications can be modeled by positive and conservative production-destruction systems (PDS) that can be expressed in the form

$$y_i'(t) = \sum_{j=1}^{N}(p_{ij}(\mathbf{y}(t)) - d_{ij}(\mathbf{y}(t))), \quad \mathbf{y}(0) = \mathbf{y}^0 \in \mathbb{R}^N_{>0}, \quad p_{ij}(\mathbf{y}), d_{ij}(\mathbf{y}) \geq 0, \quad i = 1, \ldots, N,$$

where $\mathbf{y} = (y_1, \ldots, y_N)^T$ denotes the vector of state variables. A PDS is called *positive*, if $\mathbf{y}(t) > \mathbf{0}$ holds for all $t \geq 0$, and called *conservative*, if the condition $\sum_{i=1}^N y_i(t) = \sum_{i=1}^N y_i(0)$ is satisfied for all $t \geq 0$.

For a one-step method given in the form $\mathbf{y}^{n+1} = \Phi(\mathbf{y}^n, \mathbf{y}^{n+1}, \Delta t)$ these notions translate to the conditions $y_i^{n+1} > 0$ for all $y_i^n > 0$ and positive step sizes $\Delta t > 0$ for the *unconditionally positivity*, and $\sum_{i=1}^N y_i^{n+1} = \sum_{i=1}^N y_i^n$ for all $n \in \mathbb{N}$ and $\Delta t > 0$ for the *unconditionally conservativity* of the method, respectively.

Given an explicit two-stage RK scheme with nonnegative parameters with the butcher array

$$\begin{array}{c|cc} 0 & & \\ \alpha & \alpha & \\ \hline & 1-1/(2\alpha) & 1/(2\alpha) \end{array}, \quad \alpha \geq \frac{1}{2},$$

the two-stage MPRK22(α) scheme is defined by

$$\begin{aligned} y_i^{(1)} &= y_i^n, \qquad y_i^{(2)} = y_i^n + \alpha\Delta t \sum_{j=1}^{N}\left(p_{ij}(\mathbf{y}^{(1)})\frac{y_j^{(2)}}{y_j^{(1)}} - d_{ij}(\mathbf{y}^{(1)})\frac{y_i^{(2)}}{y_i^{(1)}}\right), \\ y_i^{n+1} &= y_i^n + \Delta t \sum_{j=1}^{N}\Bigg(\left(\left(1-\frac{1}{2\alpha}\right)p_{ij}(\mathbf{y}^{(1)}) + \frac{1}{2\alpha}p_{ij}(\mathbf{y}^{(2)})\right)\frac{y_j^{n+1}}{(y_j^{(2)})^{1/\alpha}(y_j^{(1)})^{1-1/\alpha}} \\ &\qquad - \left(\left(1-\frac{1}{2\alpha}\right)d_{ij}(\mathbf{y}^{(1)}) + \frac{1}{2\alpha}d_{ij}(\mathbf{y}^{(2)})\right)\frac{y_i^{n+1}}{(y_i^{(2)})^{1/\alpha}(y_i^{(1)})^{1-1/\alpha}}\Bigg), \end{aligned}$$

for $i = 1, \ldots, N$, see [2]. MPRK schemes were first mentioned in [1], and proven to be unconditionally positive and unconditionally conservative in [2]. Whereas the MPRK22(α) method is proven to be second order accurate in [2], there are also results about third order MPRK schemes, see [3], [4].

The classical analysis based on Dahlquist's equation is not suitable due to the specific properties of the PDS. Instead, one can investigate the positive and conservative system

$$\mathbf{y}'(t) = \mathbf{A}\mathbf{y}(t), \quad \mathbf{y}(0) = \mathbf{y}^0 \in \mathbb{R}^2_{>0} \quad \text{with} \quad \mathbf{A} := \begin{pmatrix} -a & b \\ a & -b \end{pmatrix} \quad \text{and} \quad a, b > 0. \tag{1}$$

We require then that $\mathbf{y}^n \to \mathbf{y}^* := \frac{\|\mathbf{y}^0\|_1}{a+b}\binom{b}{a}$ as $n \to \infty$ in order to mimic the behavior of the exact solution.

[*] Corresponding author: email izgin@mathematik.uni-kassel.de, phone: +49 561 804 4316
[**] email kopecz@mathematik.uni-kassel.de, phone: +49 561 804 2898
[***] email meister@mathematik.uni-kassel.de, phone: +49 561 804 2890

2 Analysis of the Linearized Method

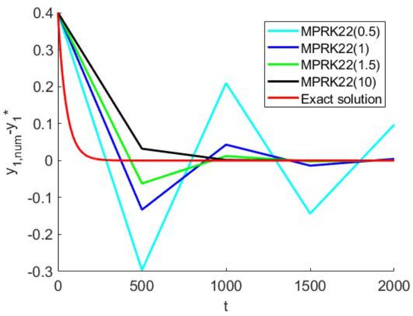
Applying the MPRK22(α) scheme to the linear test problem (1) leads to $y_i^{n+1} = f_i(\mathbf{y}^n)$ with

$$f_i(\mathbf{y}^n) = y_i^n + \Delta t \frac{h_j(\mathbf{y}^n) y_j^n - h_i(\mathbf{y}^n) y_i^n}{1 + \Delta t (h_1(\mathbf{y}^n) + h_2(\mathbf{y}^n))},$$

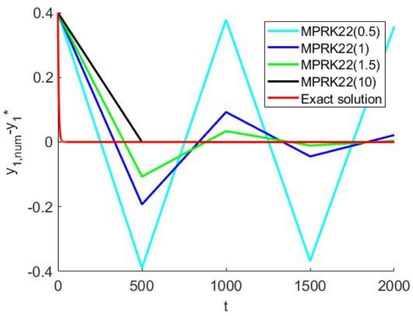
where h_1 and h_2 are nonlinear functions and $i, j \in \{1, 2\}$, $i \neq j$. The linearized method reads $\mathbf{w}^{n+1} = \mathbf{y}^* + \mathbf{Df}(\mathbf{y}^*)(\mathbf{w}^n - \mathbf{y}^*)$, $\mathbf{w}^0 := \mathbf{y}^0$, where $\mathbf{Df}$ stands for the Jacobian of $\mathbf{f}$. One then can prove that indeed, we have $\mathbf{Df}(\mathbf{y}^*)\mathbf{y}^* = \mathbf{y}^*$, and thus, end up with $\mathbf{w}^{n+1} = \mathbf{Df}(\mathbf{y}^*)\mathbf{w}^n$. One eigenvalue of the Jacobian at the stationary solution $\mathbf{y}^*$ of (1) is 1, and the other is given by the *stability function* $R(\alpha, \lambda\Delta t)$, where $\lambda := -(a + b)$ is the non-zero eigenvalue of the matrix $\mathbf{A}$ and

$$R(\alpha, z) := \frac{2 - z^2 - 2z\alpha}{2(1 - z)(1 - z\alpha)}.$$

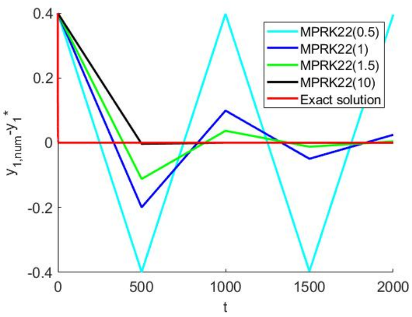
One can prove that for all $\alpha \geq \frac{1}{2}$ and all $z < 0$ we have $|R(\alpha, z)| < 1$. Hence, we can show $\mathbf{w}^n \to \mathbf{y}^*$ as $n \to \infty$ for all $\mathbf{y}_1^0, \mathbf{y}_2^0 > 0$. Indeed, analyzing $R(\alpha, z)$ results in prognoses that can be verified in numerical experiments. For instance, the larger the absolute value of z and the smaller the value of $\alpha \geq \frac{1}{2}$, the more $R(\alpha, z)$ tends to -1 which should lead to stronger oscillations. This can be seen in the following figure. However, further theory is needed in order to understand that the function R indeed leads to local convergence of the nonlinearized method.



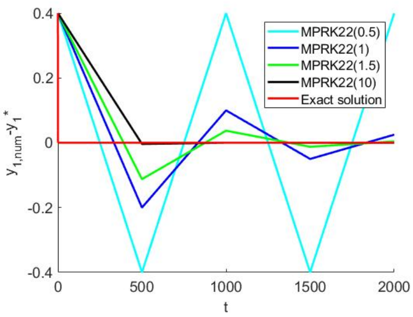
(a) $z = -10$



(b) $z = -100$



(c) $z = -1000$



(d) $z = -10000$

Fig. 1: We have chose $\Delta t = 500$, $a = b$, $z = -(a + b)\Delta t$ and compared different values of α for the MPRK22(α) method applied to (1). For the sake of simplicity we only plot first component of the numerical approximation vector $\mathbf{y}_{\text{num}}$ shifted by $\mathbf{y}_1^*$ and compare it to the shifted exact solution of (1). From the top left to the bottom right, $|z|$ is increasing by factors of 10.

Acknowledgements Open access funding enabled and organized by Projekt DEAL.

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