Communications to SIMAI Congress,
ISSN 1827-9015, Vol. 2 (2007)

DOI: 10.1685/CSC06028

On the uniform accuracy of IMEX Runge-Kutta schemes and applications to hyperbolic systems with relaxation

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Abstract. In this paper we consider new Implicit-Explicit (IMEX) Runge-Kutta schemes for hyperbolic systems of conservation laws with stiff relaxation terms. The schemes were obtained by imposing additional order conditions to guarantee better accuracy over a wide range of the stiffness parameter ε. Numerical comparisons of the new schemes with some other schemes confirm an improvement of the accuracy for small values of ε.

Key words. Runge-Kutta methods, stiff problems, hyperbolic systems with relaxation, order conditions.

AMS Subject Classification: 65C20, 65L06

1. Introduction. Several physical problems of great importance for applications are described by stiff system in the form:

$$U' = F(U) + \frac{1}{\varepsilon}G(U) \tag{1}$$

where $U = U(t) \in R^m$, F,$G : R^m \to R^m$, and $\varepsilon > 0$ is the stiffness parameter.
Systems of such form often arise from the discretization of partial differential equations, such as convection-diffusion equations, hyperbolic systems with relaxation (i.e. discrete kinetic theory of rarefied gases, hydrodynamical models for semiconductors, etc.,[2,3,4,5,7,13]), where a method of lines approach is usually used.
The development of numerical methods for systems (1) has considerably attracted a lot of attention in recent years. The goal of this paper is to develop numerical methods that work better than other IMEX Runge Kutta schemes existing in the literature. We introduce here a new class of Implicit-Explicit (IMEX) Runge-Kutta (R-K) methods suitable for time dependent partial differential systems that are able to handle the stiffness of the system (1).This work is motivated by the study of the global error for different types of IMEX R-K methods existing in literature.[9] This error analysis is accompanied by an order reduction phenomenon where the observed convergence rates of the methods drop the classical order of accuracy. The development of these methods is aided by the knowledge of new order conditions derived to impose accuracy at the various order in the stiffness parameter ε.[10] We require extra order conditions in addition to the classical order conditions presented in literature for the IMEX Runge Kutta schemes,[2,3,4,5,6].
Hence, this approach allows the construction of new uniformly accurate IMEX Runge-Kutta schemes producing an error which is more uniform in the stiffness parameter. In particular, they are used to improve some existing scheme (see also[9]). Our analysis is based on the smoothness assumption of the solution and also applies to the stiff case when $\Delta t \gg \varepsilon$ (see,[9,10]).

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The outline of the paper is as follows. In the next section we present the general structure of IMEX Runge-Kutta schemes. In section 3 we report the new order conditions up to third-order derived from.[10] In particular, we introduce two new third-order IMEX Runge-Kutta schemes, MARS(3,4,3) and MARK3(2)4L[2]SA (see[9]). Section 4 is devoted to compare the different performances of these new schemes with respect to two classical third-order IMEX Runge-Kutta schemes, ARS(3,4,3),,[6] and ARK3(2)4L[2]SA,.[2] Finally, in Section 5 we examine the results obtained. Conclusions are drawn and work in progress is mentioned.

2. IMEX Runge-Kutta Schemes and Classification. An IMEX Runge-Kutta method applied to (1) has the following form

$$U_{n+1} = U_n + h\sum_{i=1}^{s} \tilde{b}_i F(t_n + \tilde{c}_i h, U^i) + h\sum_{i=1}^{s} b_i \frac{1}{\varepsilon} G(t_n + c_i h, U^i) \tag{2}$$

with internal stages given by

$$U^i = U_n + h\sum_{j=1}^{i-1} \tilde{a}_{ij} F(t_n + \tilde{c}_i h, U^i) + \sum_{j=1}^{i} a_{ij} \frac{1}{\varepsilon} G(t_n + c_i h, U^i). \tag{3}$$

The matrices $(\tilde{a}_{ij})$, with $\tilde{a}_{ij} = 0$ for $j \geq i$, and (a_{ij}) are $s \times s$ matrices such that the resulting method is explicit in F, and implicit in G using a diagonally implicit method ($a_{ij} = 0$, for $j > i$) for G gives a sufficient condition to guarantee that F is always evaluated explicitly; furthermore, this choice is usually preferred over full implicit schemes for efficiency reasons. The methods are characterized by the coefficients vectors $\tilde{c} = (\tilde{c}_1, ..., \tilde{c}_s)^T$, $\tilde{b} = (\tilde{b}_1, ..., \tilde{b}_s)^T$, $c = (c_1, ..., c_s)^T$, $b = (b_1, ..., b_s)^T$. Then they can be represented by a double *tableau* in the usual Butcher notation,

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b}^T \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array}.$$

The coefficients $\tilde{c}$ and c, used for the treatment of non autonomous systems, are given by the usual relation

$$\tilde{c}_i = \sum_{j=1}^{i-1} \tilde{a}_{ij}, \quad c_i = \sum_{j=1}^{i} a_{ij} \tag{4}$$

The great number of IMEX R-K methods presented in literature lead us to classify these ones in three different types characterized by the structure of the matrix $A = (a_{ij})_{i,j=1}^{s}$ of implicit scheme.

Definition 1. *We call an IMEX R-K method of type A,* (see[5])*, if the matrix* $A \in \mathbb{R}^{s \times s}$ *is invertible.*

Definition 2. *We call an IMEX R-K method of type CK,* (see[2])*, if matrix* $A \in \mathbb{R}^{s \times s}$ *can be written as*

$$A = \begin{pmatrix} 0 & 0 \\ a & \hat{A} \end{pmatrix}$$

with the submatrix $\hat{A} \in \mathbb{R}^{(s-1) \times (s-1)}$ *is invertible.*

Remark. IMEX R-K methods, called of type ARS (see[6]), are a special case of the type CK with the vector $a = 0$.

3. Additional order conditions. The IMEX Runge-Kutta methods can be viewed as a particular class of partitioned Runge-Kutta methods. Therefore, their order conditions can be derived from the general theory of order conditions for partitioned methods. Order conditions for partitioned Runge-Kutta methods have been derived in.[8] For a detail account of the order conditions for the Runge-Kutta schemes see, for example,[2] and.[3] Now, in[11] we have been derived additional order conditions that, together to the classical order conditions, assure accuracy at the various order in the stiffness parameter ε We remark that in the classical literature IMEX R-K schemes do not satisfy them. Let us write explicitly the additional order conditions up to third-order. For a detail analysis we refer.[11]

Index 1 Order Conditions

$$\sum_{i,j} b_i \omega_{ij} \tilde{c}_j = 1, \sum_{i,j} b_i \omega_{ij} \tilde{c}_j^2 = 1, \sum_{i,j} b_i \omega_{ij} \tilde{a}_{ik} \tilde{c}_k = 1/2, \tag{5}$$

Index 2 Order Conditions

$$\begin{array}{ll} \sum_{i,j} b_i \omega_{ij} \omega_{jk} \tilde{c}_k^2 = 2, & \sum_{i,j,k} b_i \omega_{ij} \omega_{jk} c_k^2 = 2, \\ \sum_{i,j,k} b_i \omega_{ij} \omega_{jk} \tilde{c}_k c_k = 2, & \sum_{i,j,k,l} b_i \omega_{ij} \omega_{jk} \tilde{a}_{kl} \tilde{c}_l = 1, \\ \sum b_i \omega_{i,j} \omega_{jk} \tilde{a}_{kl} c_l = 1 & . \end{array} \tag{6}$$

Then, it may be advantageous to have schemes that satisfy these new order conditions. In fact, here we consider IMEX Runge-Kutta schemes that use the whole set of classical order conditions (see,[12] and[3]) and formulas (5). In the Tables below we collect some third-order IMEX Runge-Kutta schemes called MARK3(2)4L[2]SA and MARS(3,4,3) (see[9]).

MARK3(2)4L[2]SA scheme:

0	0	0	0	0
c_2	0.43586652150845	γ	0	0
c_3	−4.30002662176923	2.26541338346372	γ	0
1	0.60424832458800	0	0.04011484609646	γ
	b_1	0	b_3	γ

0	0	0	0	0
c_2	0.871733043016917	0	0	0
c_3	−3.06478674186224	1.46604002506519	0	0
1	0.21444560762133	0.71075364965269	0.07480074272597	0
	b_1	0	b_3	γ

$\gamma = 0.43586652150845,\ c_2 = 0.87173304301691,\ c_3 = -1.59874671679705,$
$b_1 = 0.60424832458800,\ b_3 = 0.04011484609646.$

MARS(3,4,3) scheme:

0	0	γ	0	0
c_2	0	γ	0	0
c_3	0	0.28206673924577	γ	0
1	0	1.20849664917601	−0.64436317068446	γ
	0	b_2	b_3	γ

0	0	0	0	0
c_2	0.87173304301691	0	0	0
c_3	0.535396540307354	0.182536720446875	0	0
1	0.63041255815287	−0.83193390106308	1.20152134291021	0
	0	b_2	b_3	γ

$\gamma = 0.435866521508458,\ c_2 = \gamma,\ c_3 = 0.71793326075423,$
$b_2 = 1.20849664917601,\ b_3 = -0.64436317068446.$

4. Numerical Simulations. In this section we present some numerical results obtained when we apply these new schemes to situations where hyperbolic systems with relaxation are presented. In these problems we perform an accuracy test and integrate the equations with smooth solutions.
High accuracy in space is obtained by finite difference discretization with Weighted Essentially Non Oscillatory (WENO) reconstruction,,[15,4] We remark that finite difference can be used only with uniform (or smoothly varying) mesh. Therefore, in the computations presented in this paper we use an uniform mesh and the local Lax-Friedrichs flux to evaluate the flux function. For a more detailed description about WENO reconstruction the reader can consult the review by Shu.[15]
Now we apply the new schemes to two test problems. The first test problem is a simple linear system with stiff relaxation source term[14]

$$\begin{aligned} &\partial_t u + \partial_x v = 0, \\ &\partial_t v + \partial_x u = (au - v)/\varepsilon. \end{aligned} \tag{7}$$

As $\varepsilon \to 0$ the source term describes the equilibrium equation $v = au$ and substituting this value in the second equation in (7) gives the equilibrium differential equation $\partial_t u + a\partial_x u = 0$.
We have considered a periodic smooth solution with initial *well-prepared* data that are given by $u(x,0) = sin(2\pi x)$ and $v(x,0) = v_0(x,0) + \epsilon v_1(x,0)$, where $v_0(x,0) = au(x,0)$ and $v_1(x,0)$ is the first Chapman-Enskog expansion. We set $a = 0.5$, Courant number between 0.5 and 1 and the final time is $t = 0.2$. The system is integrated for $t \in [0,2]$.
Table shows the corresponding convergence rate for the v-component (stiff component) in L_∞-norm. Different norms L_1 and L_2 give essentially the same results.

Now we apply the new schemes to the *Broadwell model* of the nonlinear Boltzmann equation, (,[7],[134]). We have considered a periodic smooth solution with initial *well-prepared*

Table 1. Convergence rate for v in L_∞-norm

Schemes	$\varepsilon = 1$	$\varepsilon = 10^{-1}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-5}$	$\varepsilon = 10^{-6}$	$\varepsilon = 10^{-8}$
ARS	3.770	3.171	2.254	1.996	1.993	1.993
MARS	3.110	3.002	2.216	3.201	3.197	3.196
ARK3	3.289	3.055	2.165	2.038	2.036	2.036
MARK3	3.105	2.999	2.216	3.204	3.200	3.200

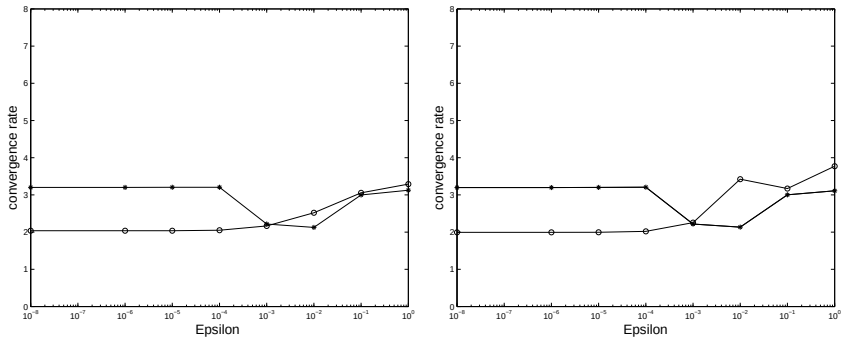


Figure 1. Convergence rate vs ε for the v-component (stiff component). ($\circ$) ARK3(2)4L[2]SA and ARS(3,4,3) scheme, ($*$) MARS(3,4,3) and MARK3(2)4L[2]SA scheme.

data given by

$$\begin{aligned}
&\rho(x,0) = 1 + a_\rho \sin\tfrac{2\pi x}{L},\\
&u(x,0) = \tfrac{1}{2} + a_v + \sin\tfrac{2\pi x}{L},\\
&m(x,0) = \rho(x,0)u(x,0),\\
&z(x,0) = z_E(\rho(x,0)m(x,0)) + \varepsilon z_1(\rho(x,0)m(x,0)).
\end{aligned}$$

where $z_1(x,0)$ is the first Chapman-Enskog expansion. In our computations we used the parameters $a_\rho = 0.3$, $a_v = 0.1$, $L = 20$ and we integrated the equations for $t \in [0, 30]$. Courant number $\Delta t/\Delta x = 0.6$ has been used.

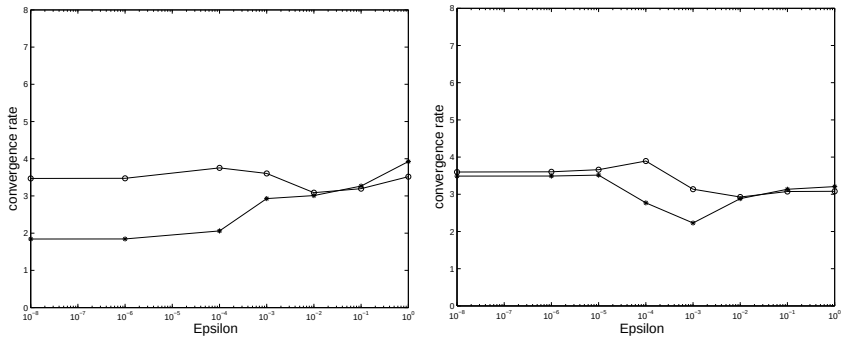


Figure 2. Convergence rate vs ε for the density ρ ($\circ$) and the flux of the momentum z ($*$). ARS(3,4,3) scheme (left) and MARS(3,4,3) scheme (right).

5. Discussion. In[9] we have proposed the MARS(3,4,3) and MARK3(2)4L[2]SA schemes to improve some IMEX Runge Kutta schemes existing in the literature (in particular ARS(3,4,3) and ARK3(2)4L[2]SA schemes) when applied to systems of ordinary differential equations. We have explicitly assumed that the coefficients of the scheme satisfy the additional order conditions (5). As we have seen, we have obtained an improvement

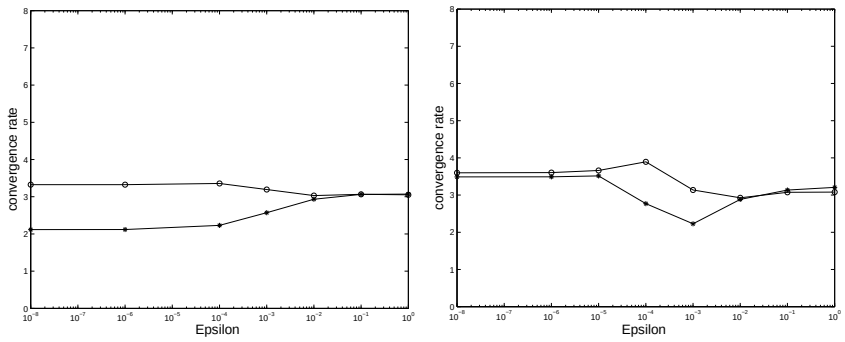


Figure 3. Convergence rate vs ε for the density ρ ($\circ$) and the flux of the momentum z ($*$). ARK3(2)4L[2]SA (left) scheme and MARK3(2)4L[2]SA scheme (right).

for the convergence of the stiff component that guarantees a uniform accuracy of the schemes for small and large values of the parameter ε. Analogously in this paper, as it is evident from the Table and Figures, the MARS(3,4,3) and MARK3(2)4L[2]SA schemes improve the convergence rate of the MARS(3,4,3) and MARK3(2)4L[2]SA schemes when applied to a systems of partial differential equations. In fact, for the first problem we increase the convergence rate for the v-component (stiff component) for sufficiently stiff parameters ($\varepsilon < 10^{-4}$), namely when $\varepsilon \to 0$. In a similar way, we have improved the convergence of variable z in the Broadwell model. Then, a third-order accuracy is observed for a small and large values of ε. Note that for intermediate values of the parameter ε ($10^{-4} < \varepsilon < 10^{-2}$) we have a slight deterioration of the accuracy. However, these results reveal that additional order conditions for the coefficients are necessary to have an IMEX Runge-Kutta scheme that works uniformly with respect to the stiffness parameter ε. In order to have uniform accuracy in ε, in[12] we shall develop such schemes satisfying the whole set of additional order conditions (5) and (6). The main goal is to perform a numerical study of the convergence rate for a wide range of ε and to check whether the convergence is uniform in ε also in the intermediate regime.

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