

LOCAL ACCURACY AND ERROR BOUNDS OF THE IMPROVED RUNGE-KUTTA NUMERICAL METHODS

Sania Qureshi, Zaib-un-Nisa Memon, Asif Ali Shaikh

*Department of Basic Sciences and Related Studies, Mehran University of Engineering and Technology
Jamshoro, Pakistan*

sania.qureshi@faculty.muett.edu.pk, zaib.memon@faculty.muett.edu.pk

asif.shaikh@faculty.muett.edu.pk

Received: 4 August 2018; Accepted: 14 December 2018

Abstract. In this paper, explicit Improved Runge-Kutta (IRK) methods with two, three and four stages have been analyzed in detail to derive the error estimates inherent in them whereas their convergence, order of local accuracy, stability and arithmetic complexity have been proved in the relevant literature. Using single and multivariate Taylor series expansion for a mathematical function of one and two variables respectively, slopes involved in the IRK methods have been expanded in order to obtain the general expression for the leading or principal term in the local truncation error of the methods. In addition to this, principal error functions of the methods have also been derived using the idea of Lotkin bounds which consequently gave rise to the error estimates for the IRK methods. Later, these error estimates were compared with error estimates of the two, three, and four-stage standard explicit Runge-Kutta (RK) methods to show the better performance of the IRK methods in terms of the error bounds on the constant step-size h used for solving the initial value problems in ordinary differential equations. Finally, a couple of initial value problems have been tested to determine the maximum absolute global errors, absolute errors at the final nodal point of the integration interval and the CPU times (seconds) for all the methods under consideration to get a better idea of how the methods behave in a particular situation especially when it comes to analyzing the error terms.

MSC 2010: 49K15, 65L05, 65L06, 65L07, 65L12.

Keywords: error estimate, remainder term, principal error function, truncation error, Lotkin bound

1. Introduction

A number of physical laws are expressed in terms of mathematical models that are based on different kinds of differential equations. Such models form an important part for the study of applied and computational mathematics. Differential equations play a vital role in the field of science and engineering. Applied mathematicians, computational analysts and researchers in the fields are the people who come into contact with such mathematical models more frequently than anyone else. Popula-

tion growth or decay in population dynamics, the Lorentz attractor model in weather prediction, mass-spring system in physics, simple and forced pendulum in mechanics, kinetic reactions in chemistry, formulation of tissues in human body in physiology, the speed of efflux in fluid dynamics, flow of current in electric circuits, change in the Gross Domestic Product (GDP) over time in economics, displacement of a beam in civil, agent-based fabric modeling in textile, heating and cooling of computer hardware in computer science, prediction of structure failures and other examples are all the indispensable applications of differential equations. These and many other applications of differential equations can be found in [1–8]. Thus, differential equations are the useful tools to model the complex behavior of the physical world. Most of these equations are too difficult to solve exactly. In other words, their closed form solution is not possible to obtain where the nonlinearity of the equations constitutes the major reason. There are many nonlinear ordinary differential equations whose exact solution cannot be found using existing analytical techniques. On the other hand, most of the linear equations can be solved in terms of elementary mathematical functions but not all. In any case, numerical methods come into play to get approximate solution of every type of important equation and the task has become comparatively easy after the advent of digital computers.

With the passage of years, several numerical methods have been designed because one method cannot serve the whole purpose. In the history of these methods, the methods called single-step linear explicit RK, multi-step explicit Adams-Bashforth, multi-step implicit Adams-Moulton, Backward Differentiation Formulae, Parallel-in-time methods and few more are known as the standard/classical numerical methods to solve the initial value problems in ordinary differential equations as can be found in [9]. Among the family of these classical methods, the fourth order explicit linear RK method is quite famous [10] for having only four slope evaluations per integration step in contrast to higher order methods which use more slope evaluations per integration step than their order of convergence as proved in [11, 12]. Further study on the analysis and importance of these RK methods is found in the work of Hull et al. [13]. It is due to this reason, Max Lotkin [14] provided a better estimate of the local error inherent in the classical RK method. In an effort of reducing slope evaluations, authors in [15–17] proposed improved versions of the classical RK methods. Nonetheless, most of these methods were employed on an autonomous type of initial value problems whereas the IRK methods with two, three and four stages devised in [18] could be used for both autonomous and non-autonomous scalar and vector-valued initial value problems thereby getting much attention of the researchers interested in the field of computational mathematics [19]. While maintaining the order of convergence p with additional an advantage of employing $p - 1$ slope evaluations per integration step in case of at least two-stage IRK3-2 methods considered in this paper, they perform much better than most of the existing classical RK methods having same number of slope evaluations per integration step. Since these methods may be used to solve various problems of practical interest in applied and computational mathematics, it seems important to have an estimate of the local truncation error and

bound for this error inherent to these methods. Like numerical accuracy of classical RK methods, the third and fourth order IRK methods are explored in detail for their local truncation errors and the numerical accuracy derived in terms of the error bounds.

The principal goal of the present paper is to get such estimate of the error and to derive a bound for the constant step-size h required by the IRK methods.

2. Material and methods

Linear explicit classical RK methods have advantageously been used to solve initial value problems in ordinary differential equations of the form:

$$\frac{dy}{dx} = f(x, y); \quad y(x_0) = y_0, \quad y, f \in R, \quad x \in [x_0, x_n] \in R \quad (1)$$

where it is assumed that the problem is well-posed, that is, it has a unique continuously differentiable solution, say $y(x)$. The notation y_n has been used to show the approximate solution to the exact solution $y(x_n)$ at the nodal points $x_n = x_0 + nh$; $n = 0, 1, 2, \dots, N$, where $h = (x_n - x_0) / N$ is called the constant step-size. Moreover, the convergent Taylor series expansion of the exact solution $y(x)$ of (1) assumed to be smooth about $x = a$ as shown below is required to agree with the IRK methods with two, three and four stages up to the terms in h^3 and h^4 respectively:

$$\begin{aligned} y(x+h) = & y(x=a) + hf + \frac{1}{2!}h^2(f_x + ff_y) + \frac{1}{3!}h^3(f_{xx} + 2ff_{xy} + f^2f_{yy} + ff_y^2 + f_xf_y) \\ & + \frac{1}{4!}h^4 \left(\begin{aligned} & f_{xxx} + f^3f_{yyy} + ff_y^3 + f_xf_y^2 + f_{xx}f_y + 5ff_yf_{xy} + 4f^2f_yf_{yy} \\ & + 3(ff_{xxy} + f^2f_{xyy} + f_xf_{xy} + ff_xf_{yy}) \end{aligned} \right) \quad (2) \\ & + \frac{1}{5!}h^5 \left(\begin{aligned} & 13ff_xf_yf_{yy} + 3f_x^2f_{yy} + 12(f^2f_{xy}f_{yy} + ff_xf_{xyy}) \\ & + 7(f_xf_yf_{xy} + f^3f_yf_{yyy}) + 11f^2f_y^2f_{yy} + 9(ff_yf_{xxy} + ff_y^2f_{xy}) \\ & + 15f^2f_yf_{xyy} + 4(ff_{xx}f_{yy} + ff_{xxy} + f^3f_{xyyy} + f^3f_y^2 + f_{xx}f_{xy}) \\ & + 8ff_{xy}^2 + 6(f^2f_xf_{yyy} + f^2f_{xxy} + f_xf_{xxy}) + f^4f_{yyyy} + ff_y^4 \\ & + f_xf_y^3 + f_{xx}f_y^2 + f_{xxx}f_y + f_{xxxx} \end{aligned} \right) + O(h^6) \end{aligned}$$

$$\text{Generally, } y(x) = \sum_{n=0}^{\infty} \frac{y^{(n)}(a)}{n!} (x-a)^n + R_n \quad (3)$$

where the remainder term $R_n \rightarrow 0$ as $n \rightarrow \infty$ for all x in the interval of convergence. This Taylor series has given rise to the standard RK methods with s number of slope evaluations per integration step and written from [9] as follows:

$$\left. \begin{aligned} y_{n+1} &= y_n + h \sum_{i=1}^s b_i k_i \\ k_1 &= f(x_n, y_n) \\ k_2 &= f(x_n + p_2 h, y_n + h q_{21} k_1) \\ &\vdots \\ k_s &= f\left(x_n + p_s h, y_n + h \sum_{j=1}^{s-1} q_{sj} k_j\right) \end{aligned} \right\} \quad (4)$$

2.1. General form of the IRK methods

The authors in [20] have described their proposed IRK methods with s number of stages having order of convergence either s or $s+1$ depending upon the higher power of the step-size h to which the slopes involved in the methods are Taylor expanded as given below:

$$\left. \begin{aligned} y_{n+1} &= y_n + h \left[b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^s b_i (k_i - k_{-i}) \right] \\ k_1 &= f(x_n, y_n); \quad k_{-1} = f(x_{n-1}, y_{n-1}) \\ k_i &= f\left(x_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j\right) \\ k_{-i} &= f\left(x_{n-1} + c_i h, y_{n-1} + h \sum_{j=1}^{i-1} a_{ij} k_{-j}\right) \\ 1 \leq n \leq N-1, \quad 2 \leq i \leq s \text{ for } c_2, \dots, c_s \in [0, 1] \\ \text{and } c_i &= \sum_{j=1}^{i-1} a_{ij} \end{aligned} \right\} \quad (5)$$

From this general structure of the IRK methods, two, three and four-stage IRK methods have been chosen in the present study for finding the error estimates and bounds inherent to them.

An accurate estimate of the error has been obtained by a comparison of the exact coefficient $1/4! f'''$ of h^4 of the Taylor expansion with the approximate one originating from (5) two and three-stage IRK methods, that is, IRK3-2 and IRK3-3 respectively. Suppose the IRK3-2 and IRK3-3 have been expressed in the following form:

$$y(x_0 + h) = y_0 + C_1 h + C_2 h^2 + C_3 h^3 + C_4 h^4 + \dots$$

where $C_i = \frac{1}{i!} y_0^{(i)}$, $i = 1, 2, 3$, and $C_4 + \varepsilon = 1/4! f'''$.

All the slopes involved in IRK3-2 have now been Taylor expanded and considering third order accuracy of the method IRK3-2, terms up to the h^3 were canceled when compared with Taylor series given by (2). Thus, we have the following leading term of the local truncation error of the method concerned:

$$\begin{aligned} \epsilon_{IRK3-2} = & \frac{1}{4!}f''' - \frac{1}{2}b_2c_2^2 \left[\begin{array}{l} 2(ff_yf_{xy} + f^2f_yf_{yy} + ff_xf_{yy} + f_xf_{xy}) \\ + 3(f^2f_{xyy} + ff_{xxy}) + f^3f_{yyy} + f_{xxx} \end{array} \right] \\ & + \frac{1}{6}[3b_2c_2 - (b_{-1} + b_2)] \left[\begin{array}{l} 5ff_yf_{xy} + 3(ff_xf_{yy} + f_xf_{xy} + f^2f_{xyy} + ff_{xxy}) \\ + f^3f_{yyy} + f_{xxx} + ff_y^3 + f_xf_y^2 + f_{xx}f_y + 4f^2f_yf_{yy} \end{array} \right] \end{aligned} \quad (6)$$

Similarly, all the slopes involved in the IRK3-3 method have been Taylor expanded and considering third order accuracy of the method, terms up to h^3 were once again canceled when compared with Taylor series given by (2). Thus, we have the following leading term of the local truncation error of the method given by IRK3-3:

$$\begin{aligned} \epsilon_{IRK3-3} = & \frac{1}{4!}f''' - \frac{1}{2}b_3 \left[\begin{array}{l} (f^3f_{yyy} + f^2f_{xyy} + 2f^2f_yf_{yy} + 2ff_xf_{yy}) \\ (a_{32}^2 + a_{31}^2 + 2a_{31}a_{32}) \end{array} \right] \\ & - \frac{1}{6}(b_2 + b_3) \left[\begin{array}{l} 5ff_yf_{xy} + 3(ff_xf_{yy} + f^2f_{xyy} + f_xf_{xy} + ff_{xxy}) \\ + f^3f_{yyy} + ff_y^3 + f_{xx}f_y + f_xf_y^3 + f_{xxx} + 4f^2f_yf_{yy} \end{array} \right] \\ & + b_3(a_{31} + a_{32}) \left[\begin{array}{l} \frac{1}{2}(f^3f_{yyy} + ff_y^3 + f_xf_y^2 + f_{xx}f_y + ff_{xxy} + 3ff_xf_{yy}) \\ + 2ff_y(f_{xy} + ff_{yy}) + f^2f_{xyy} + f_xf_{xy} \end{array} \right] \\ & - \frac{1}{2}b_3c_3^2(ff_{xy} + f_{xx}) \\ & - b_3c_3(a_{31} + a_{32})(f_xf_{xy} + f^2f_{xyy} + ff_{xxy} + ff_yf_{xy}) \\ & - \frac{1}{2}\left(\frac{1}{3}b_{-1} - b_2c_2\right) \left[\begin{array}{l} f^3f_{yyy} + ff_y^3 + f_xf_y^2 + f_{xx}f_y + f_{xxx} + 3f^2f_{xyy} \\ + 3(f_xf_{xy} + ff_{xxy} + ff_xf_{yy}) + 5ff_yf_{xy} + 4f^2f_yf_{yy} \end{array} \right] \\ & + \frac{1}{2}b_3c_3[f^2f_{xyy} + f_xf_{xy} + ff_yf_{xy} + f_{xxx} + 2ff_{xxy}] \\ & - \frac{1}{2}b_2c_2^2 \left[\begin{array}{l} f^3f_{yyy} + 3ff_{xxy} + f_{xxx} + 2 \left(\begin{array}{l} f^2f_yf_{yy} + ff_xf_{yy} + ff_yf_{xy} \\ + f^2f_{xyy} + f_xf_{xy} \end{array} \right) \end{array} \right] \\ & - b_3a_{32}c_2[f_xf_{xy} + ff_y^3 + f_xf_y^2 + f_{xx}f_y + ff_xf_{yy} + 3ff_yf_{xy} + 2f^2f_yf_{yy}] \end{aligned} \quad (7)$$

Whereas the leading term of the local truncation error of IRK4-4 method has not been mentioned for the sake of brevity. However, the leading terms of the local truncation error for the standard RK methods with two and three stages-excluding four-stage RK for the same reason - have been determined below for the comparison purpose later:

$$\epsilon_{RK2} = \frac{1}{3!}f'' - \frac{1}{2}b_2[q_{21}^2f^2f_{yy} + p_2^2f_{xx} + 2p_2q_{21}ff_{xy}]$$

$$\epsilon_{RK3} = \frac{1}{4!} f'''' - \left[\begin{array}{l} \frac{1}{6} (b_2 q_{21}^3 + 3b_3 q_{31}^2 q_{32} + 3b_3 q_{31} q_{32}^2 + b_3 q_{31}^3 + b_3 q_{32}^3) f^3 f_{yyy} + b_3 p_2 p_3 q_{32} f_x f_{xy} \\ + \frac{1}{2} (b_2 p_2 q_{21}^2 + b_3 p_3 q_{32}^2 + 2b_3 p_3 q_{31} q_{32} + b_3 p_3 q_{31}^2) f^2 f_{xyy} \\ + \frac{1}{2} (b_2 p_2^2 q_{21} + b_3 p_3^2 q_{31} + b_3 p_3^2 q_{32}) f f_{xxy} + \frac{1}{6} (b_2 p_2^3 + b_3 p_3^3) f_{xxx} \\ + \left(\frac{1}{2} b_3 q_{21}^2 q_{32} + b_3 q_{21} q_{31} q_{32} + b_3 q_{21} q_{32}^2 \right) f^2 f_y f_{yy} + \frac{1}{2} b_3 p_2^2 q_{32} f_{xx} f_y \\ + (b_3 p_2 q_{21} q_{32} + b_3 p_3 q_{21} q_{32}) f f_y f_{xy} + (b_3 p_2 q_{32}^2 + b_3 p_2 q_{31} q_{32}) f f_x f_{yy} \end{array} \right]$$

3. Error bounds

In order to achieve the required error bounds, the idea of Lotkin's bound has been used as explained in [14],

$$|f(x, y)| < M, |f_y(x, y)| < L \text{ and } \left| \frac{\partial^{i+j} f}{\partial x^i \partial y^j} \right| < \frac{L^{i+j}}{M^{j-1}};$$

where $(i + j) \leq$ order of the method, L and M are positive constants independent of x and y .

Employing the above idea, we can find a general expression for the Principal Error Function (PEF) $\psi(x, y)$ of IRK3-2, IRK3-3 and standard RK methods having the same number of stages as that of corresponding IRK methods in the form given below:

$$|\psi(x, y)|_{IRK3-2} = \left| \frac{13}{12} - \frac{13}{3} (b_{-1} + b_2) + b_2 c_2 (13 - 8c_2) \right| h^4 L^3 M$$

$$|\psi(x, y)|_{IRK3-3} = \left| \begin{array}{l} \frac{13}{12} - 3b_3 (a_{32}^2 + a_{31}^2 + 2a_{31} a_{32}) - \frac{13}{3} (b_2 + b_3) + \\ 10b_3 (a_{31} + a_{32}) - b_3 c_3^2 - 4b_3 c_3 (a_{31} + a_{32}) - \\ \frac{13}{3} (b_{-1} - 3b_2 c_2) + 3b_3 c_3 - \frac{15}{2} b_2 c_2^2 - 10b_3 a_{32} c_2 \end{array} \right| h^4 L^3 M$$

$$|\psi(x, y)|_{RK2} = \left| 1 - b_2 p_2 q_{21} - \frac{1}{2} b_2 (q_{21}^2 + p_2^2) \right| h^3 L^2 M$$

$$|\psi(x, y)|_{RK3} = \frac{13}{12} - \left[\begin{array}{l} \frac{1}{6} (b_2 q_{21}^3 + b_3 (q_{31} + q_{32})^3) + b_3 p_2 q_{32} (q_{32} + q_{31} + \frac{1}{2} p_2 + p_3) \\ + \frac{1}{2} (b_2 p_2 q_{21}^2 + b_3 p_3 (q_{31} + q_{32})^2) \\ + b_3 q_{21} q_{32} \left(\frac{1}{2} q_{21} + q_{32} + q_{32} + p_2 + p_3 \right) \\ + \frac{1}{2} (b_2 p_2^2 q_{21} + b_3 p_3^2 (q_{31} + q_{32})) + \frac{1}{6} (b_2 p_2^3 + b_3 p_3^3) \end{array} \right] h^4 L^3 M$$

All of these derived local truncation errors and their respective principal error functions of the RK and IRK methods have now been useful in comparing the error estimates resulting from these methods. It may be noted that these principal error functions specially for the IRK methods have not been previously discussed/derived in the relevant literature.

4. Numerical experiments

In this section, the error bounds and the step-size error bounds have been derived for all the IRK and the standard RK methods as mentioned above. In addition to this, a few numerical experiments have also been included to compute the errors and CPU time (seconds) values produced by the above all types of RK methods. Stability regions and convergence analysis for some of the sets of these IRK methods can be found in [18, 20] whereas the rest follows. In order to compare bounds obtained for the local truncation error and step-size h required to employ the method, given below is the Butcher form of some frequently used standard two, three and four stages RK and IRK methods for comparison of their error estimates using couple of initial value problems discussed next:

$\begin{array}{c cc} \text{RK2} & & \\ 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$	$\begin{array}{c cc} \text{IRK3-2} & & \\ 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline -1/3 & 2/3 & 5/6 \end{array}$
$\begin{array}{c ccc} \text{RK3} & & & \\ 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$	$\begin{array}{c ccc} \text{IRK3-3} & & & \\ 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 1 & -1 & 2 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$
$\begin{array}{c cccc} \text{RK4} & & & & \\ 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$	$\begin{array}{c cccc} \text{IRK4-4} & & & & \\ 0 & 0 & 0 & 0 & 0 \\ 1/5 & 1/5 & 0 & 0 & 0 \\ 3/5 & 0 & 3/5 & 0 & 0 \\ 4/5 & 2/15 & 4/25 & 38/75 & 0 \\ \hline & 19/288 & 307/288 & -25/144 & 25/144 \end{array}$

Thus, using the above mentioned Lotkin's bounds, one can find the required error bounds for the above tabulated IRK and RK methods as summarized in the following table; where tol shows the error tolerance set prior to solving the initial value problem. Values for L and M have chosen so that following conditions may be satisfied: $|f(x, y)| < M$ and to get appropriate value of L one may first compute the bounds $L_{i,j}$

Table 1. Bounds for standard RK and IRK methods

	Methods					
	IRK3-2	RK2	IRK3-3	RK3	IRK4-4	RK4
Error Bound	$\frac{8}{3}h^4L^3M$	$\frac{1}{2}h^3L^2M$	$\frac{985}{648}h^5L^4M$	$\frac{1}{12}h^4L^3M$	$\frac{1}{95}h^5L^4M$	$\frac{1}{36}h^5L^4M$
Step-size Bound	$\sqrt[4]{\frac{3 \times tol}{8 \times L^3M}}$	$\sqrt[3]{\frac{2 \times tol}{L^2M}}$	$\sqrt[5]{\frac{648 \times tol}{985 \times L^4M}}$	$\sqrt[4]{\frac{12 \times tol}{L^3M}}$	$\sqrt[5]{\frac{95 \times tol}{L^4M}}$	$\sqrt[5]{\frac{36 \times tol}{L^4M}}$

for $\left| \frac{\partial^{i+j} f}{\partial x^i \partial y^j} \right|$, then take the following quantities:

$$L_{i+j} = \max \left[\left(L_{i+j,0}/M \right)^{1/(i+j)}, \left(L_{i+j-1,1} \right)^{1/(i+j)}, \left(ML_{i+j-2,2} \right)^{1/(i+j)}, \dots, \left(M^{i+j-1} L_{0,i+j} \right)^{1/(i+j)} \right], (i+j) \leq \text{order of the method}$$

Then, we may substitute: $L = \max(L_1, L_2, L_3, L_4)$. At this stage, a couple of linear and nonlinear initial value problems have been considered to determine the bounds of the step-size length required for solving the problems. The error tolerance for these problems has been set to $\zeta = 10^{-10}$. Values for L and M have been chosen so that the above conditions may be satisfied.

Problem 1. $\frac{dy}{dx} = x + y, y(0) = 0, x \in [0, 1] (L = M = 1)$

Problem 2. $\frac{dy}{dx} = -10(y - 1)^2, y(0) = 2, x \in [0, 1] (L = 20, M = 10)$

Problem 3. $\frac{dy}{dx} = 1 + y^2, y(0) = 1, x \in [0, 1] (L = M = 2)$

Table 2. Bounds on step-size for standard RK and IRK methods for Problems 1-3

Order	Stages	Methods	$h \leq$ for IVP 1	$h \leq$ for IVP 2	$h \leq$ for IVP 3
3	2	IRK3-2	2.4746e-03	1.4714e-04	1.2373e-03
		RK2	5.8480e-04	3.6840e-05	2.9240e-04
3	3	IRK3-3	9.1966e-03	5.2821e-04	4.5983e-03
		RK3	5.8857e-03	3.4996e-04	2.9428e-03
4	4	IRK4-4	2.4862e-02	1.4280e-03	1.2431e-02
		RK4	2.0477e-02	1.1761e-03	1.0238e-02

According to results listed in the Table 2, if the step-size bound of the IRK methods with all the stages is compared with their classical RK counterpart methods, then it is easy to observe that the former require considerably fewer iterations than the latter for the IVPs listed above. For example, for the first IVP, one may use about 404 iterations for the IRK3-2 method as compared to 1710 iterations required for the classical RK2. Secondly, 109 iterations are required by the IRK3-3 method in comparison with the classical RK3 for which about 170 iterations are necessary to get the same approximate results. Finally, the IRK4-4 method needs 40 iterations in contrast to 49 by the classical RK4 and the same holds for rest of the IVPs. Henceforth, the IRK methods perform far better than the classical RK

methods having an equal number of stages when it comes to the error bounds of the local truncation errors and bounds for the constant step-size as shown in the foregoing discussion. Next, the errors and CPU times produced by the methods under discussion have been computed in order to analyze the constant step size required to approximate the solution of an initial value problem.

Problem 4. Let us consider a nonautonomous initial value problem taken from [21] as given below:

$$\frac{dy}{dx} = -\frac{xy}{1+x^2}; y(0) = 1, \text{ with exact solution } y(x) = \frac{1}{\sqrt{1+x^2}}.$$

The Tables 3, 4 and 5 show that the maximum absolute global error, absolute error at the final nodal point of the integration interval $[0, 1]$, and CPU times in seconds, respectively, against the step-size produced by the IRK methods with two, three and four stages are comparatively smaller than the errors given by standard RK methods with the same order of local accuracy having a slight exception in the CPU time values but it does no disadvantage on average.

Table 3. Maximum absolute global errors for Problem 4

h	IRK3-2	RK2	IRK3-3	RK3	IRK4-4	RK4
0.025	2.0670e-06	2.9377e-05	3.3367e-08	1.9433e-07	3.3479e-10	9.1069e-10
0.0125	2.5910e-07	7.3025e-06	2.0900e-09	2.4213e-08	2.1513e-11	5.6637e-11
0.00625	3.2428e-08	1.8205e-06	1.3074e-10	3.0216e-09	1.3544e-12	3.5314e-12

Table 4. Final absolute errors for Problem 4

h	IRK3-2	RK2	IRK3-3	RK3	IRK4-4	RK4
0.025	2.0738e-07	2.7957e-05	2.2595e-08	1.5575e-07	3.0215e-10	6.9908e-10
0.0125	2.6604e-08	6.9468e-06	1.4078e-09	1.9368e-08	1.8711e-11	4.3384e-11
0.00625	3.3655e-09	1.7315e-06	8.7830e-11	2.4145e-09	1.1680e-12	2.7018e-12

Table 5. CPU times (seconds) for Problem 4

h	IRK3-2	RK2	IRK3-3	RK3	IRK4-4	RK4
0.025	6.2500e-02	0.0000e+00	4.6875e-02	0.0000e+00	1.8750e-01	0.0000e+00
0.0125	6.2500e-02	0.0000e+00	1.5625e-01	0.0000e+00	2.3438e-01	0.0000e+00
0.00625	5.7813e-01	0.0000e+00	3.9063e-01	0.0000e+00	2.5000e-01	0.0000e+00

Problem 5. Finally, we consider system of initial value problems as given below:

$$\begin{aligned} y_1'(x) &= -2y_1 + y_2 + 2 \sin(x) \\ y_2'(x) &= y_1 - 2y_2 + 2(\cos(x) - \sin(x)) , \\ y_1(0) &= 2, y_2(0) = 3 \end{aligned}$$

with exact solution $y_1(x) = 2e^{-x} + \sin(x)$
 $y_2(x) = 2e^{-x} + \cos(x)$.

Given below, the Tables 6, 7 and 8 show that the maximum absolute global error, absolute error at the final nodal point of the integration interval $[0, 10]$ for both the

unknowns, that is, y_1 and y_2 , and CPU times for varying values of the step-size; produced by the IRK methods with two, three and four stages are comparatively smaller than the errors given by standard RK methods with the same order of local accuracy having a slight exception in the CPU time values but it once again does no disadvantage on average. Further, these errors keep decreasing with a decrease in the step-size of the methods having IRK with smaller errors at every stage.

Table 6. Errors and CPU time for Problem 5 with step size $h = 0.025$

Method	CPU Time	MaxErrory1	MaxErrory2	LastErrory1	LastErrory2
IRK3-2	8.9063e-01	7.7638e-06	1.3491e-06	1.7657e-06	1.3300e-07
RK2	1.5625e-02	9.1839e-05	6.6403e-05	2.2968e-05	4.3508e-05
IRK3-3	1.0781e+00	9.7167e-08	4.8752e-08	2.2067e-08	1.1277e-08
RK3	0.0000e+00	1.5634e-06	1.4649e-06	5.2205e-07	8.7773e-07
IRK4-4	1.4375e+00	1.7958e-08	1.2479e-08	1.3797e-08	8.3088e-09
RK4	1.5625e-02	2.5789e-08	2.6135e-08	9.0293e-09	1.1917e-08

Table 7. Errors and CPU time for Problem 5 with step size $h = 0.0125$

Method	CPU Time	MaxErrory1	MaxErrory2	LastErrory1	LastErrory2
IRK3-2	1.6875e+00	9.7351e-07	1.6616e-07	2.2138e-07	1.5590e-08
RK2	1.5625e-02	2.2644e-05	1.6328e-05	5.5131e-06	1.0686e-05
IRK3-3	2.1719e+00	6.0882e-09	3.0494e-09	1.3872e-09	7.1443e-10
RK3	0.0000e+00	1.9215e-07	1.7987e-07	6.3029e-08	1.0747e-07
IRK4-4	2.7969e+00	1.1268e-09	7.8475e-10	8.6913e-10	5.2724e-10
RK4	1.5625e-02	1.5829e-09	1.6043e-09	5.4647e-10	7.2654e-10

Table 8. Errors and CPU time for Problem 5 with step size $h = 0.00625$

Method	CPU Time	MaxErrory1	MaxErrory2	LastErrory1	LastErrory2
IRK3-2	5.1719e+00	1.2188e-07	2.0665e-08	2.7716e-08	1.8822e-09
RK2	1.5625e-02	5.6222e-06	4.0490e-06	1.3507e-06	2.6486e-06
IRK3-3	4.6719e+00	3.8099e-10	1.9066e-10	8.6959e-11	4.4958e-11
RK3	0.0000e+00	2.3815e-08	2.2283e-08	7.7421e-09	1.3296e-08
IRK4-4	6.9531e+00	7.0559e-11	4.9195e-11	5.4537e-11	3.3205e-11
RK4	1.5625e-02	9.8013e-11	9.9365e-11	3.3391e-11	4.4675e-11

5. Conclusions

In this research work, it was observed that the linear explicit IRK methods with two, three and four stages produced the error estimates smaller than the ones produced by their counterparts, that is, two, three and four-stage standard linear explicit RK methods. The principal term for the local truncation errors of the methods was derived and compared with the existing RK methods to show better performance of

the IRK methods. Thus, the IRK methods not only use reduced slope evaluations per integration step while maintaining the same order of local accuracy as that of standard RK methods but they are also a more useful measure for determining the constant step-size h required to solve an initial value problem in ordinary differential equations as was observed in Tables 1 and 2. Further, maximum absolute global errors and the absolute errors at the final nodal point for IRK methods are also smaller than those produced by the standard RK methods as shown in the above tabular data. Based upon the bounds derived above, it is concluded that the IRK methods are computationally more effective as they require a smaller number of iterations to approximate the solution of an initial value problem in comparison with standard linear explicit RK type methods.

Acknowledgement

The authors are highly thankful to anonymous reviewer(s) for their suggestions to improve the first version of the present research paper. The authors are also grateful to the Mehran University of Engineering and Technology, Jamshoro, Pakistan to provide the facilities to carry out this research work.

References

- [1] Qureshi, S., Shaikh, A.A., & Chandio, M.S. (2013). A new iterative integrator for Cauchy problems. *Sindh University Research Journal-SURJ (Science Series)*, 45(3).
- [2] Bird, J. (2017). *Higher Engineering Mathematics*. London: Routledge.
- [3] Mahata, A., Roy, B., Mondal, S.P., & Alam, S. (2017). Application of ordinary differential equation in glucose-insulin regulatory system modeling in fuzzy environment. *Ecological Genetics and Genomics*, 3, 60-66.
- [4] Qureshi, S., Shaikh, A.A., & Chandio, M.S. (2015). Critical study of a nonlinear numerical scheme for initial value problems. *Sindh University Research Journal-SURJ (Science Series)*, 47(4).
- [5] Qureshi, S., Chandio, M.S., Junejo, I.A., Shaikh, A.A., & Memon, Z.U.N. (2014). On error bound for local truncation error of an explicit iterative algorithm in ordinary differential equations. *Science International*, 26(2).
- [6] Davis, M.E. (2013). *Numerical methods and modeling for chemical engineers*. Courier Corporation.
- [7] Zill, D.G. (2012). *A first course in differential equations with modeling applications*. Cengage Learning.
- [8] Qureshi, S., & Ramos, H. (2018). L-stable explicit nonlinear method with constant and variable step-size formulation for solving initial value problems. *International Journal of Nonlinear Sciences and Numerical Simulation*, 19(7-8), 741-751.
- [9] Butcher, J.C. (2016). *Numerical Methods for Ordinary Differential Equations*. John Wiley & Sons.
- [10] Musa, H., Saidu, I., & Waziri, M.Y. (2010). A simplified derivation and analysis of fourth order Runge Kutta method. *International Journal of Computer Applications*, 9(8), 51-55.
- [11] Khaliq, A.Q.M. (1983). *Numerical Methods for Ordinary Differential Equations* (Doctoral dissertation). Department of Mathematics and Statistics, Brunel University Uxbridge, Middlesex, England.

-
- [12] Qureshi, S., Sandilo, H., Sheikh, H., & Shaikh, A. (2016). Local truncation error and associated principal error function for an iterative integrator to solve Cauchy problems. *Science International*, 28(4).
- [13] Hull, T.E., Enright, W.H., & Jackson, K.R. (1996). Runge-Kutta Research at Toronto. *Applied Numerical Mathematics*, 22(1), 225-236.
- [14] Lotkin, M. (1951). On the accuracy of Runge-Kutta's method. *Mathematical Tables and Other Aids to Computation*, 5(35), 128-133.
- [15] Goeken, D., & Johnson, O. (1999). Fifth-order Runge-Kutta with higher order derivative approximations. *Electronic Journal of Differential Equations*, 2(November), 1-9.
- [16] Ismail, M.M. (2011). Goeken-Johnson Sixth-Order Runge-Kutta Method. *Journal of Education and Science*, 24(49), 119-128.
- [17] Goeken, D., & Johnson, O. (2000). Runge-Kutta with higher order derivative approximations. *Applied Numerical Mathematics*, 34(2-3), 207-218.
- [18] Rabiei, F., & Ismail, F. (2011). *New Improved Runge-Kutta Method with Reducing Number of Function Evaluations*. International Conference on Software Technology and Engineering, 3rd (ICSTE 2011). ASME Press.
- [19] Ansari, M.Y., Shaikh, A.A., & Qureshi, S. (2018). Error bounds for a numerical scheme with reduced slope evaluations. *J. Appl. Environ. Biol. Sci.*, 8, 67-76.
- [20] Rabiei, F., Ismail, F., & Suleiman, M. (2013). Improved Runge-Kutta methods for solving ordinary differential equations. *Sains Malaysiana*, 42(11), 1679-1687.
- [21] Udawadia, F.E., & Farahani, A. (2008). Accelerated Runge-Kutta Methods. *Discrete Dynamics in Nature and Society*, 2008.