Full Length Research Paper

Numerical treatment of Kap's equation using a class of fourth order method

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Kap's equation is a stiff initial value problem. This paper deals with the treatment of Kap's equation using a class of 4th order explicit Runge–Kutta method. Numerical computation was carried out using Microsoft Visual C++. The results of the computation were found to be highly accurate and consistent with minima errors. A comparison of the results generated from the scheme was also carried out vis-a-vis some other conventional explicit Runge–Kutta formulae. The proposed class of method was found to compare favourably well.

Key words: Kap's equation, stiffness, initial value problems, multiderivative explicit Runge-Kutta method, fourth-order method.

INTRODUCTION

Many fields of application, notably chemical engineering and control theory, yield Initial Value Problems (IVPs) involving systems of ordinary differential equations of the form,

$$\left. \begin{array}{l} y'(x) = f(x, y(x)), x \in [x_0, x_{end}], \\ y(x_0) = y_0. \end{array} \right\} \quad (1)$$

Where the derivative function $f : \mathbb{R} \times \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is assumed to be sufficiently continuous. There are two main classes of methods for the discretization of such problems, so-called Runge-Kutta methods and Linear Multistep Methods (Hairer et al., 2009; Hairer and Wanner, 2010; Soetaert et al., 2010).

At times, these IVPs exhibit a phenomenon known as stiffness. Stiffness occurs for instance if a problem has components with different rates of variation according to the independent variable. Very often there will be a trade off between using explicit methods that require little work per integration step and implicit methods which are able to take larger integration steps, but need (much) more work for one step (Soetaert et al., 2010). Lambert (1991), gave five propositions about stiffness, each of them capturing some important aspect of it (Brugnano et al., 2011).

The notion of stiffness, which originated in several applications of a different nature, has dominated the activities related to the numerical treatment of differential problems for the last fifty years (Brugnano et al., 2011). There are many definitions and approaches to stiffness in the literature (Brugnano et al., 2011; Griffiths and Higham, 2010; Johnson, 2010). For the purpose of this current work we narrow down on the definition of Hairer and Wanner (1996, 2010), which states that "Stiff equations are problems for which explicit methods do not work".

Many algorithms have been designed for the treatment of stiff ODEs. Sekar (2006); Sekar et al. (2004), presented RK-Butcher algorithm. He found out that discrete solutions using the RK-Butcher algorithm are found to be very accurate and are comparable with the exact solutions of the linear and nonlinear stiff problems

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and also with the Runge-Kutta method based on arithmetic mean (RKAM). Savcenco et al. (2007), introduced a multirate procedure with automatic partitioning and step size control. This scheme allows the integration of different solution components with different time steps, especially for large, stiff systems of ODEs where some components may show a more active behaviour than the others. Hundsdorfer and Savcenco (2009), proposed the θ-method with one level of temporal refinement for a simplified situation. Other works on multirate schemes can be found in Gear and Wells (1984) and Günther et al. (2001). In Beck et al. (2010), Schmitt and Weiner (2004), Podhaisky et al. (2005), Weiner et al. (2009) and Schmitt et al., (2005a, 2005b), peer methods have been applied to this class of problems. Backward differentiation formulae are another popular approach with stiff ODEs (Yatim et al., 2010; Ibrahim et al., 2008, 2007a, 2007b).

Kap's equation is an example of IVPs that exhibits stiffness. Attempts to use the classical explicit Runge-Kutta methods to solve such problems encountered very substantial difficulties. In practice, implicit methods are usually employed to advance the solution of these types of problems. Logg (2003a, 2003b) proposed an algorithm based on finite elements which is also similar to fully implicit Runge-Kutta methods in implementation. However, the cost of implementation of implicit methods is very high. This gave rise to the development of explicit methods that could still cope, to an extent, with such IVPs.

Recently, a class of explicit approximation algorithm was developed for IVPs (Akanbi et al., 2008). This family of methods is called Multiderivative Explicit Runge-Kutta (MERK) Methods. This paper presents the application of a 2-stage MERK method to nonlinear stiff IVPs using Kap's equation as a case study (Sekar, 2006; Lambert, 1991). Numerical computations show that the class of method is accurate, efficient and it competes well with some standard methods.

EXPLICIT RUNGE–KUTTA METHODS

Explicit Runge–Kutta methods are generally known to be one-step schemes. One advantage of ERK methods (and other one-step methods) is their self-starting nature (Butcher, 2003, 2009). We shall stay close to the spirit of ERK methods, yet attain higher order of accuracy by incorporating higher order derivatives of f (That is y').

As it is well known, one-step method is of the form:

$$y_{n+1} - y_n = \Phi(x_n, y_n; h) \tag{2}$$

The Taylor's algorithm of order p is obtained from (2) by

setting

$$
\begin{aligned}
\Phi(x_n, y_n; h) &= \Phi_T(x_n, y_n; h) \\
&= \sum_{r=0}^{\infty} \frac{h^{r+1}}{(r+1)!} \left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \right)^r f(x, y).
\end{aligned}
\tag{3}
$$

and whenever f does not depend on x explicitly, we have the incremental function

$$
\Phi_T(y_n; h) = \sum_{r=0}^{\infty} \frac{h^{r+1}}{(r+1)!} \left(\frac{\partial}{\partial y} \right)^r f(y).
\tag{4}
$$

An s-stage ERK method is of the form:

$$y_{n+1} - y_n = \Phi_{RK}(x_n, y_n; h) \tag{5}$$

Where

$$\Phi_{RK}(x_n, y_n; h) = \sum_{r=1}^{s} b_r K_r \tag{6}$$

$$K_1 = hf(x, y) \tag{7}$$

$$K_r = hf\left(x + c_r h, y + \sum_{u=1}^{r-1} a_{ru} K_r\right), r = 2, 3, ..., s \tag{8}$$

$$c_r = \sum_{u=1}^{r-1} a_{ru} , \ r = 2, 3, ..., s \tag{9}$$

The matrix representation of the ERK methods stated in Equations (5) – (9) is of the form:

$$
\begin{bmatrix} A & c \\ b^T & 0 \end{bmatrix} =
\begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1\,s} & a_{1\,s+1} \\
a_{21} & & & & \vdots \\
\vdots & & & & \vdots \\
a_{s1} & & \cdots & a_{ss} & a_{s\,s+1} \\
a_{s+1\,1} & & \cdots & a_{s+1\,s} & 0
\end{bmatrix}
\tag{10}
$$

These coefficients are specified as follows:

$$a_{r\,s+1} = c_r, \qquad r = 1(1)s \tag{11}$$

$$a_{s+1\,u} = b_u, \qquad u = 1(1)s \tag{12}$$

$$a_{s+1\,s+1} = 0, \qquad\qquad . \tag{13}$$

$$a_{j\,u} = a_{u\,j}, \ j, u = 1(1)s \tag{14}$$

The basis of derivation of ERK schemes is to equate the coefficients of the incremental functions $\Phi_T(x_n, y_n; h)$ and $\Phi_{RK}(x_n, y_n; h)$ to $O(h^p)$ for a p-th order method.

A CLASS OF 2–STAGE MERK METHOD OF ORDER 4

Traditionally, given an IVP (1), classical ERK methods are derived with the intention of performing multiple evaluations of $f(y)$ in each internal stage for a given accuracy. However, the new scheme is derived with the notion of incorporating higher order derivatives of $f(y)$. The cost of internal stage evaluations is reduced greatly and there is an appreciable improvement on the attainable order of accuracy of the method.

The general form of a 2–stage MERK method for an autonomous system is given as,

$$y_{n+1} - y_n = \Phi_{MERK}(y_n; h) \tag{15}$$

Where

$$\Phi_{MERK}(y_n; h) = \sum_{r=1}^{s} b_r K_r, \quad s = 2 \tag{16}$$

and we define the internal stages K_1 and K_2 as

$$K_1 = hf(y) \tag{17}$$

$$K_2 = hf\left(y + a_{21}K_1 + ha_{22}f_y K_1 + \frac{1}{2}h^2 a_{23}\left(f_y^2 + ff_{yy}\right)K_1\right) \tag{18}$$

The coefficients of h and its higher powers in the Taylor's expansion (4) and the MERK incremental function (16) were compared to obtain the values of the parameters in (16) and (18). A family of schemes called MERK methods emerged that are of orders 3 and 4 (Akanbi et al, 2008). This family of methods is a new improvement to any standard 2-stage ERK methods. Previously, a 2-stage ERK method can only give at most an order 2 scheme. But by these newly derived MERK scheme, the method can attain order 4 for a family of 2-stage methods. Indeed, an s–stage method could attain order 2s, thereby the order generated doubles the stage of the method.

A fourth order member of this family that is of interest to us in obtaining the numerical solution of Kap's equation is,

$$\left.\begin{array}{l} y_{n+1} = y_n + \frac{1}{4}K_1 + \frac{3}{4}K_2 \\[2mm] K_1 = hf(y_n) \\[2mm] K_2 = hf\left(y_n + \frac{2}{3}K_1 + \frac{2}{9}hf_y K_1 + \frac{1}{9}h^2\left(f_y^2 + ff_{yy}\right)K_1\right) \end{array}\right\} \tag{19}$$

and it is simply refer to as MERK subsequently.

We represent this scheme in Butcher array as follows:

$$\begin{bmatrix} 0 & 0 \\ \frac{2}{3} & 0 \\ \hline \frac{2}{9} & 0 \\ \frac{1}{9} & 0 \\ \hline \frac{1}{4} & \frac{3}{4} \end{bmatrix}$$

EXISTENCE AND UNIQUENESS OF SOLUTION

Not all problems possess a unique solution or indeed any solution at all. It is then worthwhile to first examine if the IVP possesses certain important properties. The following standard theorem known as existence and uniqueness theorem lays down sufficient conditions for a unique solution to exist; we shall always assume that the hypotheses of this theorem are satisfied by (1)

Theorem 1

Let $f(y)$, where $f : \mathbb{R}^n \to \mathbb{R}^n$, be defined and continuous for all (x, y) in the region D defined by $a \leq x \leq b, -\infty < y < \infty$, where a and b are finite, and let there exist a constant L such that

$$\| f(y) - f(\hat{y}) \| \leq L \| y - \hat{y} \| \tag{20a}$$

holds for every $(x, y), (x, \hat{y}) \in D$. Then for any $\eta \in \mathbb{R}^n$, there exists a unique solution $y(x)$ of the (1), where $y(x)$ is continuous and differentiable for all $(x, y) \in D$.

The requirement (20) is known as *Lipschitz condition*, and the constant L as a *Lipschitz constant*.

The following lemma will be useful for establishing the aforementioned characteristics.

Lemma 1

Let $\{\partial_i = 0(1)n\}$ be a set of real useful numbers. If there exist finite constants Γ and Π such that:

$$|\partial_{i+1}| \Gamma |\partial_i| + \Pi, \quad i = 0(1)n - 1 \tag{20b}$$

$$|\delta_i| \le \frac{\Gamma^i - 1}{\Gamma - 1}\Pi + \Gamma^i|e_0|, \quad \Gamma \ne 1. \tag{20}$$

Proof

When i = 0, (23) is satisfied identically as $|e_0| \le |e_0|$.
Suppose (23) holds whenever $i \le j$ so that

$$|\delta_j| \le \frac{\Gamma^j - 1}{\Gamma - 1}\Pi + \Gamma^j|e_0|. \tag{21}$$

Then, from (22) *i = j* implies that

$$|\delta_{j+1}| \le \Gamma|e_j| + \Pi. \tag{22}$$

On substituting (23) into (24), we have

$$|\delta_{j+1}| \le \frac{\Gamma^{j+1} - 1}{\Gamma - 1}\Pi + \Gamma^{j+1}|e_0|. \tag{23}$$

Hence, (22) holds for all *i ≥ 0*

ACCURACY AND STABILITY

Usually, during the implementation of a computational scheme, errors are generated. The magnitude of the error determines how accurate and stable a scheme is. For instance, if the magnitude of the error is sufficiently small, the computational results would be accurate. However, if the magnitude of the error becomes so large, it can make the method unstable. The sources of error for these schemes and their principal error functions are discussed in Lambert (1973, 1991); Lee (2004) and Butcher (2003). The following theorem guarantees the stability of the MERK methods.

Theorem 2

Suppose the IVP (1) satisfies the hypotheses of Theorem 2, then the new MERK algorithm is stable.

Proof

Let y_n and z_n be two sets of solutions generated recursively by the MERK method with the initial condition $y(x_0) = y_0$, $z(x_0) = z_0$, $|y_0 - z_0| = \delta_0$.

Let

$$\delta_n = y_n - z_n, \quad n \ge 0, \tag{24}$$

And

$$y_{n+1} = y_n + h\Phi_{MERK}\left(x_n, y_n; h\right), \tag{25}$$

$$z_{n+1} = z_n + h\Phi_{MERK}\left(x_n, z_n; h\right). \tag{26}$$

This implies that

$$y_{n+1} - z_{n+1} = y_n - z_n + h\left\{\Phi_{MERK}\left(x_n, y_n; h\right) - \Phi_{MERK}\left(x_n, z_n; h\right)\right\}. \tag{27}$$

Using (26) and triangle inequality, we have

$$|\delta_{n+1}| \le (1 + hL)|\delta_n|, \quad n \ge 0. \tag{28}$$

If we assume $\Gamma = 1 + hL$, and $\Pi = 0$, then Lemma 1 implies that

$$|\delta_n| \le K|\delta_0|, \tag{29}$$

Where

$$K = e^{L(b-a)} < \alpha,$$

Which implies the stability of the MERK methods.

CONVERGENCE

For a difference approximation to be usable for a class of functions $f(y(x_n))$, it is necessary that any function in this class satisfies a number of requirements as mentioned earlier on (Lambert, 1991). One of such requirement is the convergence of the method. Though convergence is implied by the consistency condition proved above. However, a succinct overview of the test of convergence is presented below:

Lemma 2

Suppose the IVP (1) satisfies the hypothesis of the Existence and Uniqueness Theorem, then the increment function Φ_{MERK} specified by (16) satisfies a Lipschitz condition of order 4 with respect to the independent variable *y*.

Proof

Suppose L is the Lipschitz constant for $f(y)$ w.r.t. *y* and

$$K_1(y_n) = hf(y_n) \tag{30}$$

Then

$$|K_1(y_n) - K_1(z_n)| = |hf(y_n) - hf(z_n)| \quad , \tag{31}$$

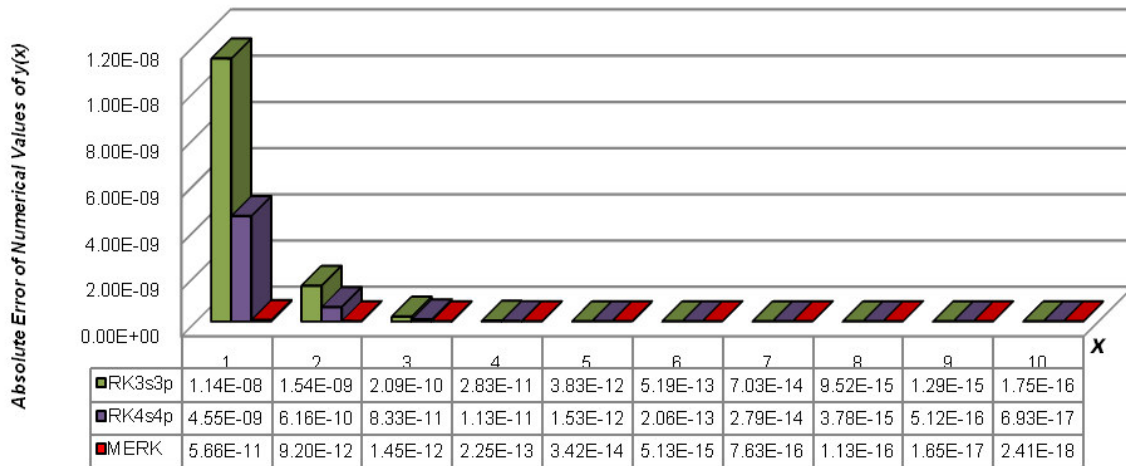$$< hL|y_n - z_n|. \tag{32}$$

Similarly,

Figure 1. Absolute Error of y(x) in the Kap's Equation for x = 0 (0.001) 10.

$$|K_2(y_n) - K_2(z_n)| = \left| hf\left(y_n + a_{21}K_1 + a_{22}hf_y(y_n)K_1 + \tfrac{1}{2}a_{23}h^2\left(f_y^2 + ff_{yy}\right)K_1\right)\right.$$

$$\left. - hf\left(z_n + a_{21}K_1 + a_{22}hf_z(z_n)K_1 + \tfrac{1}{2}a_{23}h^2\left(f_z^2 + ff_{zz}\right)K_1\right)\right| \tag{33}$$

$$< hL|y_n - z_n| + h|a_{21}|\left|K_1(y_n) - K_1(z_n)\right| + h^2|a_{22}|\left|f_yK_1(y_n) - f_zK_1(z_n)\right|$$

$$+ \tfrac{1}{2}h^3|a_{23}|\left|\left(f_y^2 + ff_{yy}\right)K_1(y_n) - \left(f_z^2 + ff_{zz}\right)K_1(z_n)\right|. \tag{33}$$

$$< L|y_n - z_n|\left\{h + h^2|a_{21}| + h^3|a_{22}| + h^4|a_{23}|\right\}. \tag{34}$$

The increment function Φ_{MERK} also implies that

$$\left|\Phi_{MERK}(y_n; h) - \Phi_{MERK}(z_n; h)\right| = |b_1K_1(y_n) + b_2K_2(y_n) - b_1K_1(z_n) - b_2K_2(z_n)|$$

$$< |b_1||K_1(y_n) - K_1(z_n)| + |b_2||K_2(y_n) - K_2(z_n)|$$

$$< hL|b_1||y_n - z_n| + L|b_2||y_n - z_n|\left\{h + h^2|a_{21}| + h^3|a_{22}| + h^4|a_{23}|\right\}$$

$$< L|y_n - z_n|\left\{(|b_1| + |b_2|)h + |b_2|\left(h^2|a_{21}| + h^3|a_{22}| + h^4|a_{23}|\right)\right\}$$

$$< L^*|y_n - z_n|, \tag{35}$$

Where the Lipschitz constant L^* is given as

$$L^* = L\left\{(|b_1| + |b_2|)h + |b_2|\left(h^2|a_{21}| + h^3|a_{22}| + h^4|a_{23}|\right)\right\}. \tag{36}$$

Thus, the proposed method is convergent to $O(h^4)$.

NUMERICAL EXPERIMENT–KAP'S EQUATION

Kap's equation is a nonlinear stiff system described by the equations: (Sekar, 2005, Lambert, 1991).

$$\left.\begin{array}{l} y'(x) = -1002y(x) + 1000z^2(x), \\[2mm] z'(x) = y(x) - z(x)\left(1 + z(x)\right), \\[2mm] y(0) = 1, \quad z(0) = 1. \end{array}\right\} \tag{37}$$

The exact solution of (40) is: $y(x) = exp(-2x)$, $z(x) = exp(-x)$. (38)

A Program code in Microsoft Visual C++ was written to solve this stiff IVP for $x \in [0, 10]$, using the MERK methods and two other conventional ERK methods. The results are displayed in Figures 1 to 4.

Two other conventional methods (Lambert 1991, 1973; Fatunla, 1988) implemented and compared with the MERK methods are stated below:

1. 3–stage scheme (RK3s3p).
$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ \tfrac{1}{3} & 0 & 0 & \tfrac{1}{3} \\ 0 & \tfrac{2}{3} & 0 & \tfrac{2}{3} \\ \tfrac{1}{4} & 0 & \tfrac{3}{4} & 0 \end{bmatrix} \tag{39}$$

2. 4–stage scheme (RK4s4p).
$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ \tfrac{1}{2} & 0 & 0 & 0 & \tfrac{1}{2} \\ 0 & \tfrac{1}{2} & 0 & 0 & \tfrac{1}{2} \\ 0 & 0 & 1 & 0 & 1 \\ \tfrac{1}{6} & \tfrac{2}{6} & \tfrac{2}{6} & \tfrac{1}{6} & 0 \end{bmatrix} \tag{40}$$
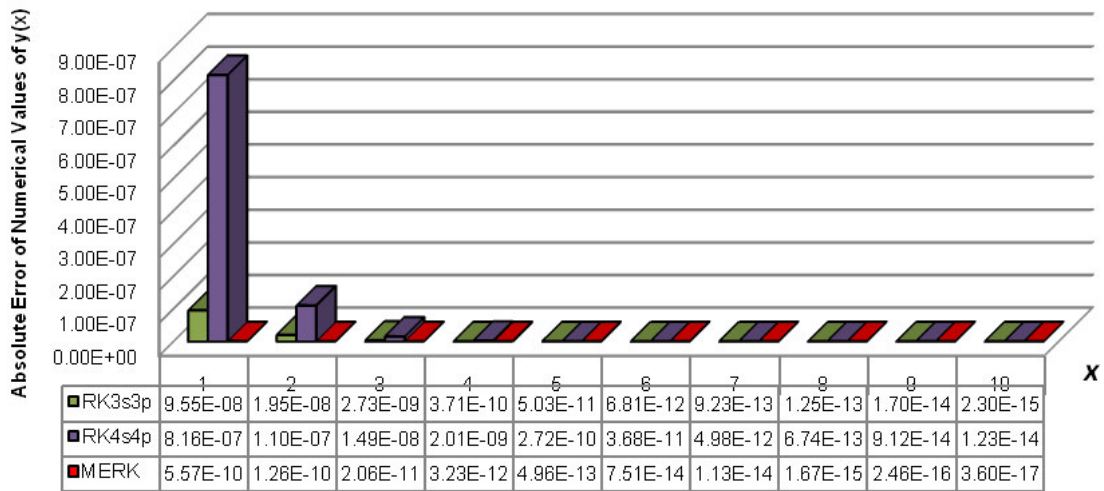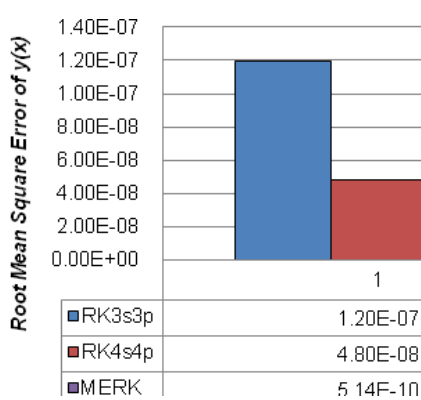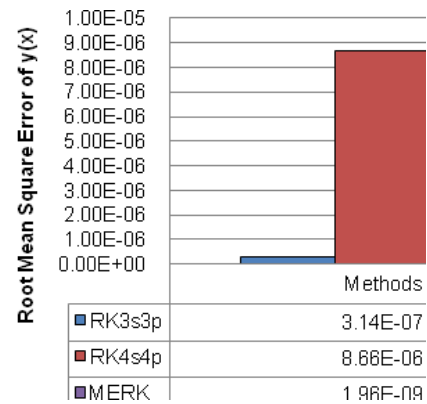
	1	2	3	4	5	6	7	8	9	10
RK3s3p	9.55E-08	1.95E-08	2.73E-09	3.71E-10	5.03E-11	6.81E-12	9.23E-13	1.25E-13	1.70E-14	2.30E-15
RK4s4p	8.16E-07	1.10E-07	1.49E-08	2.01E-09	2.72E-10	3.68E-11	4.98E-12	6.74E-13	9.12E-14	1.23E-14
MERK	5.57E-10	1.26E-10	2.06E-11	3.23E-12	4.96E-13	7.51E-14	1.13E-14	1.67E-15	2.46E-16	3.60E-17

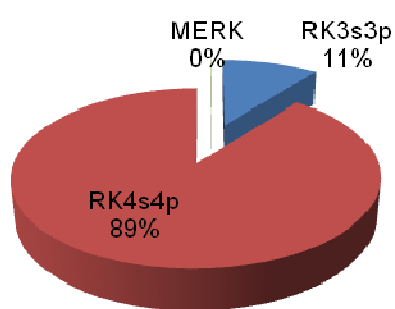**Figure 2.** Absolute Error of y(x) in the Kap's Equation for x = 0 (0.0025) 10.

	1
RK3s3p	1.20E-07
RK4s4p	4.80E-08
MERK	5.14E-10

(a) x = 0(0.001)10

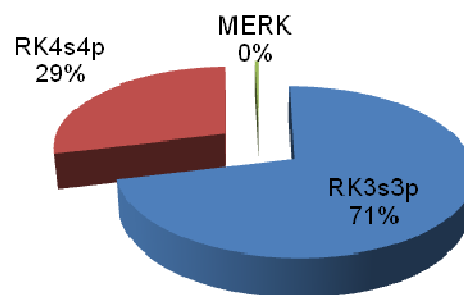|	Methods
RK3s3p	3.14E-07
RK4s4p	8.66E-06
MERK	1.96E-09

(b) x = 0(0.0025)10

Figure 3. Root Mean Square Error of y(x) in the Kap's Equation.

(a) x = 0(0.001)10

(b) x = 0(0.0025)10

Figure 4. Exploded pie chart of absolute error of y(x) in the Kap's equation.

These schemes are 3-stage order 3 and 4-stage order 4 respectively.

CONCLUSION

The results of the computation were found to be highly accurate and consistent with minima errors in the solution of Kap's equation. The comparison between the numerical values generated by these methods with the theoretical solution show that these new scheme compare favourably well and appear to possess higher order of accuracy than the existing ERK methods of orders 3 and 4. The comparison of the results is displayed in Figures 1 to 4.

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