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Error Propagation in the RK5GL3 Method

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***Abstract*—**The RK5GL3 method is a numerical method for solving initial value problems in ordinary differential equations, and is based on a combination of a fifth-order Runge-Kutta method and 3-point Gauss-Legendre quadrature. In this paper we describe the propagation of local errors in this method, and show that the global order of RK5GL3 is expected to be six, one better than the underlying Runge-Kutta method.

***Keywords*—**RK5GL3, RKrGLm, Runge-Kutta, Gauss-Legendre, initial value problem, order, local error, global error.

I. Introduction

One-step methods, such as Runge-Kutta (RK) methods, are popular methods for solving initial value problems in ordinary differential equations numerically. Of interest in such methods is the propagation of approximation error, and the cumulative effect of this propagation. In an RK method, the accumulation of $O\left(h^{r+1}\right)$ local errors results in a global error of $O\left(h^{r}\right)$, where h is the stepsize. In other words, the global order of an RK method is one less than its local order. We have developed a method [1], designated RKrGLm, which is a combination of an RK method of global order r, and m-point Gauss-Legendre (GL) quadrature, that has the interesting property that if the underlying RK method is $O\left(h^{r+1}\right)$ in its local error, then the associated RKrGLm method is $O\left(h^{r+1}\right)$ in its *global* error, i.e. the global error in RKrGLm has the same order as the local RK error. In this paper we describe error propagation specifically in the RK5GL3 method, and show the mechanism by which the global error of RK5GL3 achieves sixth order. For the benefit of the reader, a brief description of RKrGLm is given in the next section.

II. Terminology and relevant concepts

A. One-step methods

We denote an explicit RK method for solving

$$y' = f(x,y) \qquad y(x_0) = y_0 \qquad a \leqslant x \leqslant b \tag{1}$$

by

$$w_{i+1} = w_i + h_i F(x_i, w_i) \tag{2}$$

where $h_i \doteqdot x_{i+1} - x_i$ is a stepsize, w_i denotes the numerical approximation to $y(x_i)$ and $F(x,y)$ is a function associated with the particular RK method.

For example, the tableau

$$\begin{array}{lc|ccccc}
k_1: & 0 & & & & & \\
k_2: & \frac{1}{4} & \frac{1}{4} & & & & \\
k_3: & \frac{3}{8} & \frac{3}{32} & \frac{9}{32} & & & \\
k_4: & \frac{12}{13} & \frac{1932}{2197} & -\frac{7200}{2197} & \frac{7296}{2197} & & \\
k_5: & 1 & \frac{439}{216} & -8 & \frac{3680}{513} & -\frac{845}{4104} & \\
k_6: & \frac{1}{2} & -\frac{8}{27} & 2 & -\frac{3544}{2565} & \frac{1859}{4104} & -\frac{11}{40} \\
\hline
 & & \frac{16}{135} & 0 & \frac{6656}{12825} & \frac{28561}{56430} & -\frac{9}{50} & \frac{2}{55}
\end{array}$$

has

$$F(x,y) = \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6 \tag{3}$$

and corresponds to the fifth-order explicit Runge-Kutta method derived by Fehlberg [2], and is the RK method used in RK5GL3. Note that an explicit Runge-Kutta method of order r has global error $O\left(h^{r}\right)$ and local error $O\left(h^{r+1}\right)$ [3]. We use h here as a generic symbol for the stepsize. We denote the Fehlberg method described here by RK5.

B. Local and global errors

We define the global error in a numerical solution at x_i by

$$\Delta_i \doteqdot w_i - y_i, \tag{4}$$

and the local error at x_i by

$$\varepsilon_{i+1} \doteqdot [y_i + h_i F(x_i, y_i)] - y_{i+1} \tag{5}$$

In the above, y_i denotes the true solution $y(x_i)$. Note the use of the exact value y_i in the bracketed term in (5).

C. Error propagation in a one-step method

We describe a known result that is useful in our later discussion. We have

$$\begin{aligned}
w_1 &= y_0 + h_0 F(x_0, y_0) && (6)\\
\Rightarrow \Delta_1 &= y_0 + h_0 F(x_0, y_0) - y_1 && (7)\\
&= \varepsilon_1, && (8)
\end{aligned}$$

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and

$$\begin{aligned} w_2 &= w_1 + h_1 F(x_1, w_1) && (9)\\ \Rightarrow y_2 + \Delta_2 &= [y_1 + \Delta_1] + h_1 F(x_1, y_1 + \Delta_1) && (10)\\ &= [y_1 + \Delta_1] + h_1 F(x_1, y_1) \\ &\quad + h_1 \Delta_1 F_y(x_1, \xi_1) && (11)\\ \Rightarrow \Delta_2 &= [y_1 + h_1 F(x_1, y_1) - y_2] \\ &\quad + \Delta_1 [1 + h_1 F_y(x_1, \xi_1)] && (12)\\ &= \varepsilon_2 + \alpha_1 \varepsilon_1. && (13) \end{aligned}$$

Furthermore,

$$\Delta_3 = \varepsilon_3 + \alpha_2 \varepsilon_2 + \alpha_2 \alpha_1 \varepsilon_1 \quad (14)$$

and

$$\Delta_4 = \varepsilon_4 + \alpha_3 \varepsilon_3 + \alpha_3 \alpha_2 \varepsilon_2 + \alpha_3 \alpha_2 \alpha_1 \varepsilon_1 \quad (15)$$

where

$$\begin{aligned} \alpha_k &= 1 + h_k F_y(x_k, \xi_k) && (16)\\ \xi_k &\in (y_k, y_k + \Delta_k). && (17) \end{aligned}$$

In general

$$\Delta_n = \sum_{j=1}^{n} \left[\left(\frac{1}{\alpha_n} \right) \left(\prod_{k=j}^{n} \alpha_k \right) \right] \varepsilon_j. \quad (18)$$

If $|h_k F_y(x_k, \xi_k)|$ is small then $\alpha_k \approx 1$, and so

$$\Delta_n \approx \sum_{j=1}^{n} \varepsilon_j \quad (19)$$

but this is generally not expected to be the case, particularly if $F_y(x_k, \xi_k)$ is large. Furthermore, if the α's have magnitude larger than one, then the term in ε_1 could make the most significant contribution to the global error.

Since $\varepsilon_j = O\left(h^{r+1}\right)$, the global error Δ_n is the accumulation of local errors, as in

$$\Delta_n = \sum_{j=1}^{n} \beta_j h^{r+1} = \left(\frac{1}{n} \sum_{j=1}^{n} \beta_j \right) (nh) h^r = \overline{\beta} (b - a) h^r \quad (20)$$

where β_j and $\overline{\beta}$ have been implicitly defined, and we have used $nh = b - a$ (so that, in this expression, h is the average separation of the nodes x_j). Note that Δ_n is $O(h^r)$.

D. Gauss-Legendre quadrature

Gauss-Legendre (GL) quadrature on $[u, v]$ with m nodes is given by [4]

$$\int_u^v f(x, y)\, dx = h \sum_{i=1}^{m} C_i f(x_i, y_i) + O\left(h^{2m+1}\right) \quad (21)$$

where the nodes x_i are the roots of the mth degree Legendre polynomial on $[u, v]$. Here, h is the average separation of the nodes on $[u, v]$, a notation we will adopt from now on, and

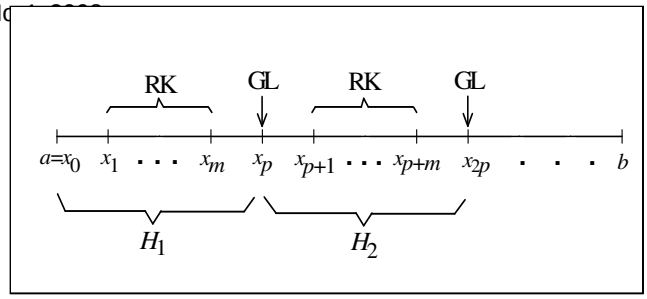

Fig. 1. RKGL algorithm for the first two subintervals H_1 and H_2 on $[a, b]$.

the C_i are appropriate weights. For GL3, the roots of the 3rd degree Legendre polynomial on $[-1, 1]$ are

$$\begin{aligned} \widetilde{x}_1 &= -0.77459666924148, \quad \widetilde{x}_2 = 0, && (22)\\ \widetilde{x}_3 &= 0.77459666924148 && (23) \end{aligned}$$

and are mapped to corresponding nodes x_i on $[u, v]$ via

$$x_i = \frac{1}{2} \left[(v - u) \widetilde{x}_i + u + v \right]. \quad (24)$$

Also, the average node separation on $[-1, 1]$ is $1/2$, and so h on $[u, v]$ is given by

$$h = \frac{1}{2} \left(\frac{v - u}{2} \right), \quad (25)$$

while the weights

$$C_1 = \frac{10}{9}, \quad C_2 = \frac{16}{9}, \quad C_3 = \frac{10}{9} \quad (26)$$

are constants on any interval of integration.

E. The RKrGLm algorithm

We briefly describe the general RKrGLm algorithm [1] on the interval $[a, b]$, with reference to Figure 1.

Subdivide $[a, b]$ into N subintervals H_i. At the RK nodes we use RKr :

$$w_{i+1} = w_i + h_i F(x_i, w_i) \quad (27)$$

At the GL nodes we use m-point GL quadrature:

$$w_{2p} = w_p + h \sum_{i=1}^{m} C_i f(x_i, w_i) \quad (28)$$

Note that $p \doteqdot m + 1$.

The GL component is motivated by

$$\begin{aligned} \int_{x_p}^{x_{2p}} f(x, y)\, dx &= y_{2p} - y_p \approx h \sum_{i=1}^{m} C_i f(x_i, y_i) && (29)\\ \Rightarrow y_{2p} &\approx y_p + h \sum_{i=1}^{m} C_i f(x_i, y_i). && (30) \end{aligned}$$

Of course, in RK5GL3 we have $r = 5, m = 3$ and $p = 4$ in the above. The RKrGLm algorithm has been shown to be consistent, convergent and zero-stable [1].

F. Local error at the GL nodes

The local error at the GL nodes is defined in a similar way to that for a one-step method:

$$\int_{x_p}^{x_{2p}} f(x,y)\,dx = \underbrace{y_{p+m+1}}_{2p} - y_p \quad (31)$$

$$= h\sum_{i=1}^{m} C_i f(x_i,y_i) + O\left(h^{2m+1}\right) \quad (32)$$

$$\Rightarrow \varepsilon_{2p} = \underbrace{\left[y_p + h\sum_{i=p+1}^{p+m} C_i f(x_i,y_i)\right]}_{\text{exact values of } y(x)} - y_{2p} \quad (33)$$

$$= O\left(h^{2m+1}\right). \quad (34)$$

Recall that $x_{2p} = x_{p+m+1}$ in the upper limit of the integral. In RK5GL3, the local error at the GL nodes is $O\left(h^7\right)$.

G. Implementation of RK5GL3

There are a few points regarding the implementation of RK5GL3 that need to be discussed:

- If we merely sample the solutions at the GL nodes, treating the computations at the RK nodes as if they were the stages of an ordinary RK method, then RK5GL3 would be reduced to an inefficient one-step method. This is not the intention behind the development of RK5GL3; rather, RK5GL3 represents an attempt to improve the efficiency of RK5, simply by replacing the computation at every fourth node by a quadrature formula which does not require evaluation of any of the stages in the underlying RK5 method.
- Of course, it is clear from the above that on H_1 the RK nodes are required to be consistent with the nodes necessary for GL quadrature. If, however, the RK nodes are located differently (perhaps due to a local error control mechanism, for example) then it is a simple matter to construct a Hermite interpolating polynomial of degree seven (which has an eighth order error) using the solutions at the nodes $\{x_0,\ldots,x_3\}$. Then, assuming x_0 maps to -1 and x_3 maps to the Legendre polynomial root $\widetilde{x}_3$ on $[-1,1]$, the position of the other nodes $\{x_1^*, x_2^*\}$ suitable for GL quadrature may be determined, and the Hermite polynomial may be used to find approximate solutions of order six at these nodes, thus facilitating the GL component of RK5GL3. A similar process is carried out on the next subinterval H_2, and so on.
- If the underlying RK5 method possesses a continuos extension it would not be necessary to construct the Hermite polynomial described above. However, there is no guarantee that a continuous extension of appropriate order (at least six, the same as the local order at the RK nodes) will be available, and it is generally true that determining a continuous extension for an RK method requires additional stages, which would most likely compromise the gain in efficiency offered by RK5GL3. Note that the construction of the Hermite polynomial does not require any additional evaluations of $f(x,y)$.

III. Error propagation in the RKGL method

In the theory that follows, we assume that the RK nodes are located as required for GL quadrature, and that the use of a Hermite polynomial, as mentioned above, is unnecessary.

A. Error propagation

For RK5GL3 we have

$$\Delta_1 = \varepsilon_1, \quad \Delta_2 = \varepsilon_2 + \alpha_1\varepsilon_1, \quad (35)$$

$$\Delta_3 = \varepsilon_3 + \alpha_2\varepsilon_2 + \alpha_2\alpha_1\varepsilon_1 \quad (36)$$

$$w_4 = y_4 + \Delta_4 \quad (37)$$

$$= y_0 + h\sum_{i=1}^{3} C_i f(x_i,w_i) \quad (38)$$

$$= y_0 + h\sum_{i=1}^{3} C_i f(x_i,y_i+\Delta_i) \quad (39)$$

$$= y_0 + h\sum_{i=1}^{3} C_i f(x_i,y_i) + h\sum_{i=1}^{3} C_i f_y(x_i,\zeta_i)\Delta_i \quad (40)$$

$$= y_0 + h\sum_{i=1}^{3} C_i f(x_i,y_i) + h\sum_{i=1}^{3}\gamma_i\varepsilon_i \quad (41)$$

$$= y_0 + h\sum_{i=1}^{3} C_i f(x_i,y_i) + A_{1,3}h \quad (42)$$

$$\Rightarrow \Delta_4 = \left[y_0 + h\sum_{i=1}^{3} C_i f(x_i,y_i) - y_4\right] + A_{1,3}h \quad (43)$$

$$= \underbrace{\varepsilon_4}_{O(7)} + \underbrace{A_{1,3}h}_{O(7)} \quad (44)$$

where $\zeta_i \in (y_i, y_i+\Delta_i)$, and $A_{1,3}$ has been implicitly defined. Also,

$$\Delta_5 = \varepsilon_5 + \alpha_4\Delta_4 \quad (45)$$

$$\Delta_6 = \varepsilon_6 + \alpha_5\varepsilon_5 + \alpha_5\alpha_4\Delta_4 \quad (46)$$

$$\Delta_7 = \varepsilon_7 + \alpha_6\varepsilon_6 + \alpha_6\alpha_5\varepsilon_5 + \alpha_6\alpha_5\alpha_4\Delta_4 \quad (47)$$

so that

$$\begin{aligned}
w_8 &= y_8 + \Delta_8 && (48)\\
&= w_4 + h\sum_{i=5}^{7} C_i f(x_i, w_i) && (49)\\
&= y_4 + \Delta_4 + h\sum_{i=5}^{7} C_i f(x_i, y_i + \Delta_i) && (50)\\
&= y_4 + \Delta_4 \\
&\quad + h\sum_{i=5}^{7} \left[C_i f(x_i, y_i) + C_i f_y(x_i, \zeta_i)\Delta_i\right] && (51)\\
&= y_4 + h\sum_{i=5}^{7} C_i f(x_i, y_i) + A_{5,7}h \\
&\quad + B_8\Delta_4 h + \Delta_4 && (52)\\
\Rightarrow \Delta_8 &= \left[y_4 + h\sum_{i=5}^{7} C_i f(x_i, y_i) - y_8\right] \\
&\quad + A_{5,7}h + B_8\Delta_4 h + \underbrace{\varepsilon_4 + A_{1,3}h}_{\Delta_4} && (53)\\
&= \underbrace{(\varepsilon_8 + \varepsilon_4)}_{O(7)} + \underbrace{(A_{5,7}h + A_{1,3}h)}_{O(7)} + \underbrace{B_8\Delta_4 h}_{O(8)}. && (54)
\end{aligned}$$

where $A_{5,7}$ and B_8 are defined below in (58) and (62). Furthermore,

$$\begin{aligned}
\Delta_{12} &= \underbrace{(\varepsilon_{12} + \varepsilon_8 + \varepsilon_4)}_{O(7)} \\
&\quad + \underbrace{(A_{9,11}h + A_{5,7}h + A_{1,3}h)}_{O(7)} \\
&\quad + \underbrace{B_{12}\Delta_8 h}_{O(8)} + \underbrace{B_8\Delta_4 h}_{O(8)}. && (55)
\end{aligned}$$

and

$$\begin{aligned}
\Delta_{16} &= \underbrace{(\varepsilon_{16} + \varepsilon_{12} + \varepsilon_8 + \varepsilon_4)}_{O(7)} \\
&\quad + \underbrace{(A_{13,15}h + A_{9,11}h + A_{5,7}h + A_{1,3}h)}_{O(7)} \\
&\quad + \underbrace{B_{16}\Delta_{12}h}_{O(8)} + \underbrace{B_{12}\Delta_8 h}_{O(8)} + \underbrace{B_8\Delta_4 h}_{O(8)}. && (56)
\end{aligned}$$

In general,

$$\begin{aligned}
\Delta_{4N} &= \underbrace{(\varepsilon_{4N} + \cdots + \varepsilon_4)}_{O(7)} + \underbrace{(A_{4N-3,4N-1}h + \cdots + A_{1,3}h)}_{O(7)} \\
&\quad + \underbrace{\left(B_{4N}\Delta_{4(N-1)}h + \cdots + B_8\Delta_4 h\right)}_{O(8)} && (57)
\end{aligned}$$

In the above, $A_{1,3}, A_{5,7}, A_{9,11}, A_{4N-3,4N-1}, B_8, B_{12}$ and B_{16} are appropriate coefficients (defined below), and N is the total number of subintervals into which $[a, b]$ has been subdivided. We list below some relevant terms in detail.

$$\begin{aligned}
A_{4N-3,4N-1} &= \sum_{i=4N-3}^{4N-1} \gamma_i\varepsilon_i. && (58)\\
\gamma_{4N-3} &= (1 + \alpha_{4N-3} + \alpha_{4N-3}\alpha_{4N-2}) \\
&\quad \cdot C_{4N-3} f_y\left(x_{4N-3}, \zeta_{4N-3}\right). && (59)\\
\gamma_{4N-2} &= (1 + \alpha_{4N-2}) \\
&\quad \cdot C_{4N-2} f_y\left(x_{4N-2}, \zeta_{4N-2}\right). && (60)\\
\gamma_{4N-1} &= C_{4N-1} f_y\left(x_{4N-1}, \zeta_{4N-1}\right). && (61)
\end{aligned}$$

$$\begin{aligned}
B_8 &= C_5 f_y(x_5, \zeta_5)\alpha_4 + C_6 f_y(x_6, \zeta_6)\alpha_4\alpha_5 \\
&\quad + C_7 f_y(x_7, \zeta_7)\alpha_4\alpha_5\alpha_6. && (62)\\
B_{12} &= C_9 f_y(x_9, \zeta_9)\alpha_8 + C_{10} f_y(x_{10}, \zeta_{10})\alpha_8\alpha_9 \\
&\quad + C_{11} f_y(x_1, \zeta_1)\alpha_8\alpha_9\alpha_{10}. && (63)\\
B_{16} &= C_{13} f_y(x_{13}, \zeta_{13})\alpha_{12} + C_{14} f_y(x_{14}, \zeta_{14})\alpha_{12}\alpha_{13} \\
&\quad + C_{15} f_y(x_{15}, \zeta_{15})\alpha_{12}\alpha_{13}\alpha_{14}. && (64)
\end{aligned}$$

In general,

$$\begin{aligned}
B_{4N} &= C_{4N-3} f_y\left(x_{4N-3}, \zeta_{4N-3}\right)\alpha_{4N-4} \\
&\quad + C_{4N-2} f_y\left(x_{4N-2}, \zeta_{4N-2}\right)\alpha_{4N-4}\alpha_{4N-3} \\
&\quad + C_{4N-1} f_y\left(x_{4N-1}, \zeta_{4N-1}\right) \\
&\quad \cdot \alpha_{4N-4}\alpha_{4N-3}\alpha_{4N-2}. && (65)
\end{aligned}$$

As for writing the global error in terms of the local errors consider, for example, Δ_{12}. Using the above expressions, we have, in terms of the local errors ε_i,

$$\Delta_{12} = \sum_{i=1}^{12} G_i\varepsilon_i \qquad (66)$$

where

$$\left.\begin{array}{ll}
G_i = \gamma_i h + (B_{12}\gamma_i + B_8\gamma_i)h^2 & \\
\quad + B_{12}B_8\gamma_i h^3 & (i = 1, 2, 3)\\
G_4 = 1 + (B_{12} + B_8)h + B_8 h^2 & \\
G_i = \gamma_i h + B_{12}\gamma_i h^2 & (i = 5, 6, 7)\\
G_8 = 1 + B_{12}h & \\
G_i = \gamma_i h & (i = 9, 10, 11)\\
G_{12} = 1 &
\end{array}\right\} \qquad (67)$$

The global error at the RK nodes is understood with reference to section 2.3 and equations (35), (36), (45)−(47).

B. Error accumulation

We have

$$\begin{aligned}
\Delta_{4N} &= \underbrace{(\varepsilon_{4N} + \cdots + \varepsilon_4)}_{O(7)} + \underbrace{(A_{4N-3,4N-1}h + \cdots + A_{1,3}h)}_{O(7)} \\
&\quad + \underbrace{\left(B_{4N}\Delta_{4(N-1)}h + \cdots + B_8\Delta_4 h\right)}_{O(8)} && (68)\\
&= NPh^7 + NQh^8 && (69)\\
&= \left(\frac{P}{4}\right)h^6\left[4Nh\right] + \left(\frac{Q}{4}\right)h^7\left[4Nh\right] && (70)\\
&= \left[\frac{P(b-a)}{4}\right]h^6 + \left[\frac{Q(b-a)}{4}\right]h^7 && (71)\\
&= O\left(h^6\right) && (72)
\end{aligned}$$

where P and Q are appropriate coefficients. This demonstrates the $O\left(h^6\right)$ character of the global error in RK5GL3.

IV. Comments

The mechanism for the $O\left(h^6\right)$ global error in RK5GL3 is shown in the first two terms on the rhs of (68). The first of these is the sum of the GL local errors which, through a suitable choice of m, is of seventh order. The second term is a linear combination of the RK local errors, multiplied by a factor h. Since each RK local error is of sixth order, this term is of seventh order. The effect of the GL component, then, is to increase the order of the accumulated RK local errors by one. We refer to this as a "quenching" effect that occurs at the GL nodes, and it serves to prevent the accumulation of the RK local errors. The third term in (68) contains terms of order eight and higher, as shown, for example, in the expansion of Δ_{12} via (66) and (67).

V. Numerical example

By way of an example, we solve the test problem

$$y' = \frac{y}{4}\left(1 - \frac{y}{20}\right) \tag{73}$$

on $[0, 5]$ with $y(0) = 1$, using RK5GL3 and RK5. This equation has solution

$$y(x) = \frac{20}{1 + 19e^{-x/4}} \tag{74}$$

and is one of the test problems used by Hull *et al* [5]. The global error is shown in Figure 2. In the upper plot the RK nodes are consistent with the nodes required for GL quadrature. In the lower plot, the RK nodes are equispaced and the RK5GL3 employs a Hermite polynomial, as described previously.The accumulation of error in RK5 is clear, whereas the error quenching in RK5GL3 is also apparent. The quenching effect occurs at each of the GL nodes, where there is clearly a sharp reduction in the magnitude of the error. In between the GL nodes the error accumulates, as expected of the RK5 method. When the RK nodes are equispaced, the RK error on the first subinterval H_1 is less than that of RK5GL3, but thereafter the superior order of RK5GL3 becomes apparent.

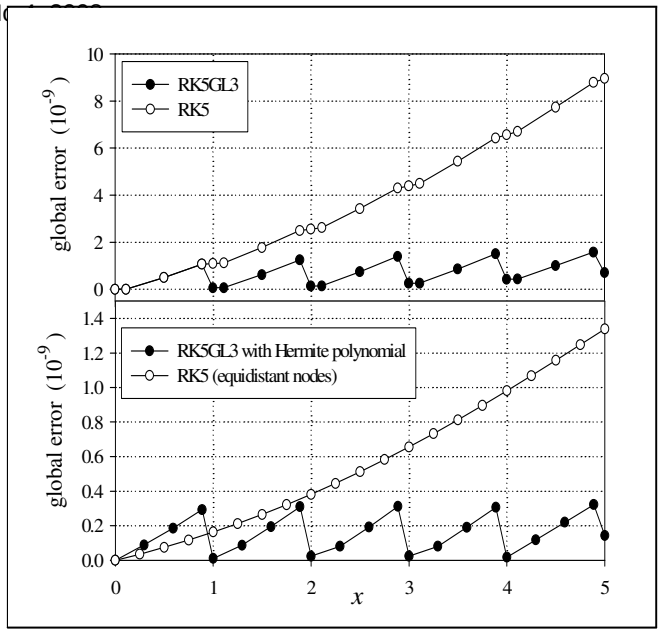

Fig. 2. Error curves for RK5GL3 and RK5 for the test problem. Upper plot has RK nodes consistent with GL quadrature. Lower plot has equidistant RK nodes, and RK5GL3 uses a Hermite polynomial, as described in the text.

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