

**R-Stable Embedded DIRKN Method of Orders 4(3) for Solving Special Second Order IVPs**

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*Abstract*

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*In this paper, we construct embedded diagonally implicit Runge-Kutta- Nystrom (DIRKN) methods of orders 4(3) for the numerical solution of the special second order initial value problems (IVPs) of the differential equation  $y'' = f(x, y)$  possessing oscillatory solutions. The motivation for this work comes from the fact that not much work seems to have been done on the embedded implicit RKN methods compared to the explicit case. In the present consideration, we derive coefficients of the method with minimized truncation error coefficients and show that it is R-stable.*

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**Keywords:** Runge-Kutta-Nystrom methods, numerical analysis, special second-order IVPs, oscillatory solutions.

**1.0 Introduction**

Consider the special second order initial value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \tag{1.1}$$

the characteristic feature here is that the function  $f$  does not explicitly depend on the first derivative  $y'$ , see [9]. This special differential equations of the second order and in particular systems of such equations occur frequently e.g. in mechanical problems without dissipation. It is often advantageous ([4], [6], [5] and [14]) to apply a direct method for this type of differential equation rather than rewriting (1.1) to its first-order form of twice the dimension and solved using the standard Runge-Kutta (RK) method.

A notable direct numerical method for the special second order initial value problem (1.1) is the Runge-Kutta-Nystrom (RKN) method. The general RKN method for equation (1.1), see for example ([8] and [14]) is of the form

$$\begin{aligned} y_{n+1} &= y_n + hy'_n + h \sum_{j=1}^s b_j F_j \\ y'_{n+1} &= y'_n + h \sum_{j=1}^s b'_j F_j \\ F_j &= f \left( x_n + c_j h, y_n + c_j h y'_n + h^2 \sum_{k=1}^s a_{jk} F_k \right) \end{aligned} \tag{1.2}$$

where the RKN parameters  $a_{kj}$ ,  $b_j$ ,  $b'_j$  and  $c_j$  are assumed to be real and  $a_{jk}$  are the stage weights,  $b_j$  weights and  $c_j$  the nodes. In most methods, the  $c_j$  satisfy

$$\frac{1}{2}c_j^2 = \sum_{k=1}^s a_{jk} \quad (j=1, \dots, s) \quad (1.3)$$

By defining the method parameters as follows

$$A = \{a_{jk}\}, \quad b = b_j, \quad b' = b'_j, \quad c = c_j,$$

the method (1.2) is compactly represented by means of the Butcher Tableau

Table 1.1: Butcher Tableau for RKNM

$c$	$A$		
			$b^T$
		$b'^T$	

RKN methods are divided into two broad classes: explicit ( $a_{jk} = 0, k \geq j$ ) and implicit ( $a_{jk} = 0, k > j$ ). The later contains the class of diagonally implicit Runge-Kutta-Nystrom (DIRKN) methods for which the  $a_{jj}$  are equal.

A number of numerical methods for this class of problems of the explicit types have been extensively discussed in numerous papers (e.g. [2], [3], [4], [5], [6], [7], [12], [14] and [17]). However, little seems to have been done on the embedded implicit methods. The particular examples in [13] and [15] are the implicit cases of the methods, but are not embedded.

In this paper, we will derive embedded implicit method of orders 4(3), which is a four-Stage diagonally implicit RKN method for the special second order IVPs in (1.1)

## 2.0 The Embedded RKN Methods

An efficient implementation must allow for variable step size. This will enable us to estimate the local truncation error at each step and control it by taking a step size such that the local error is less than some prescribed tolerance. It is usual to achieve this by identifying an embedded method of lower order in the underlying methods. Generally, efficient RKN methods involved the embedded pairs of orders  $q(p)$ , where the method of order  $q = p + 1$  used to obtain the numerical solution of the problem and the method of order  $p$  is used obtain the local truncation error, which is used for feeding the step size control algorithm. Hence the algorithm developed here is the variable step size algorithm.

The idea is to construct RKN formulae with themselves contain besides the numerical approximation  $y_{n+1}$ ,  $y'_{n+1}$ , a second approximation  $\hat{y}_{n+1}$ ,  $\hat{y}'_{n+1}$  to  $y(x_{n+1})$  and  $y'(x_{n+1})$  according to

$$\begin{aligned} y_{n+1} &= y_n + hy'_n + h^2 \sum_{j=1}^s b_j F_j, & y'_{n+1} &= y'_n + h \sum_{j=1}^s b'_j F_j \\ \hat{y}_{n+1} &= y_n + hy'_n + h^2 \sum_{j=1}^s \hat{b}_j F_j, & \hat{y}'_{n+1} &= \hat{y}'_n + h \sum_{j=1}^s \hat{b}'_j F_j \\ F_j &= f\left(x_n + c_j h, y_n + c_j h y'_n + h^2 \sum_{k=1}^s a_{jk} F_k\right) \end{aligned} \quad (2.1)$$

such that both use the same function values. The first two formulae are of order  $q$  and the second two are of order  $p$ ,  $s$  denotes the number of function evaluations that are needed for each step,  $h$  is the step size.

The differences  $y_{n+1} - \hat{y}_{n+1}$  and  $y'_{n+1} - \hat{y}'_{n+1}$  yields an estimate of the leading term of the local truncation error and can be used for step size control. The formula commonly used for variable step-size, see [4] and [5] is

$$h_{n+1} = 0.9h_n \left[ \frac{T}{\left( \max \left\{ \|\Delta_{n+1}\|_\infty, \|\Delta'_{n+1}\|_\infty \right\} \right)} \right]^{\frac{1}{(p+1)}}$$

$$h_{n+1} = 0.9h_n \left[ \frac{T}{\left( \max \left\{ \|\Delta_{n+1}\|_\infty, \|\Delta'_{n+1}\|_\infty \right\} \right)} \right]^{\frac{1}{(p+1)}}$$

where  $\Delta_{n+1} = y_{n+1} - \hat{y}_{n+1} = h^2 \sum_{j=1}^s (b_j - \hat{b}_j) F_j$

$$\Delta'_{n+1} = y'_{n+1} - \hat{y}'_{n+1} = h \sum_{j=1}^s (b'_j - \hat{b}'_j) F_j$$

are the absolute values of the largest of the truncation error terms,  $h_{n+1}$  the current step size,  $h_n$  is the size of the previous step and T is the approximate value of the desired accuracy (tolerance). If the estimated step  $h_{n+1}$  produces truncation error that are larger than T, the step should be recomputed with a smaller value of  $h_{n+1}$ . When this difficulty repeatedly occurs, the factor 0.9 should be decreased.

### 3.0 Stability of RKN Method

In studying linear stability of DIRKN methods, we use the standard test problem

$$y'' = \omega^2 y, (\omega > 0) \tag{3.1}$$

when (1.2) is applied to (3.1) we obtain the following recursive relation

$$y_{n+1} = y_n + h y'_n - z b^T Y_n$$

$$h y'_{n+1} = h y'_n - z b'^T Y_n$$

where

$$z = -h^2 \omega^2, \quad Y_n = (y_n e + h y'_n e) N^{-1}, \quad N = I + zA$$

$$e = (1, L, 1)^T, \quad c = (c_1, L, c_s)^T.$$

Eliminating the auxiliary vector  $Y_n$  yields

$$R(z) = \begin{bmatrix} 1 + z b^T (I - zA)^{-1} e & 1 + z b^T (I - zA)^{-1} c \\ z b'^T (I - zA)^{-1} e & 1 + z b'^T (I - zA)^{-1} c \end{bmatrix} \tag{3.2}$$

This matrix  $R(z)$  which determines the stability of the method is called the amplification matrix.

Introducing the functions

$$s(z) = \text{Trace}(R(z)) \quad \text{and} \quad p(z) = \text{Det}(R(z)) \tag{3.3}$$

the characteristic equation corresponding to equation (3.2) is of the form.

$$\zeta^2 - s(z)\zeta + p(z) = 0 \tag{3.4}$$

If  $\rho(R)$  denotes the spectral radius of  $R(z)$ , method (1.2) is said to be R-stable if  $\rho(R) \leq 1$  for all  $z < 0$  and the eigenvalues on the unit disk are simple. This means the amplitude of the numerical solution (3.1) does not increase with time for all  $\omega$  and  $h$ .

If  $\rho(R) = 1$  for all  $z < 0$ , method (1.2) is said to be p-stable, and if (1.2) is R-stable and  $\rho(R) \rightarrow 0$  as  $z \rightarrow -\infty$ , the method is said to be RL-stable. The interval  $(z_0, 0)$  ( $z_0 < 0$ ) on which  $\rho(R) \leq 1$  is called the interval of stability, see [2] and [13]. The method parameters of the embedded DIRKN formula

*Journal of the Nigerian Association of Mathematical Physics Volume 16 (May, 2010), 169 - 180*

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would have to be chosen so that it is either R-stable or its stability matrix has bounded eigen-values, see [13]. According to [16], the eigenvalues of (3.2) which are the zeros of (3.4) are on the unit disc if

$$\begin{aligned}
 R_1(z) &= 1 - \rho(z) \geq 0 \\
 R_2(z) &= \rho(z) + 1 - s(z) \geq 0 \\
 R_3(z) &= \rho(z) + 1 + s(z) \geq 0
 \end{aligned}
 \tag{3.5}$$

The feature of a non-empty interval of periodicity is important in integrating periodic solution. It guarantees that for  $z \in (z_0, 0)$ , the numerical solution will not be damped (or amplified),  $z_0$  is called the stability boundary.

**Definition** ([8]): A Nystrom method (1.2) has order  $p$  if for sufficiently smooth problems (1.1)

$$y(x_0 + h) - y_1 = O(h^{p+1}), \quad y'(x_0 + h) - y'_1 = O(h^{p+1})$$

For RKN method to be of order  $p$ , it must satisfy certain order conditions. The order conditions for formulae of types (1.2) have been presented by [1], [6] and [8].

#### 4. Derivation of the Embedded DIRKN Method

For a process with  $S = 4$ ,  $q = 4$  and  $\rho = 3$ , we have to satisfy seventeen order conditions (see e.g. [13] and [14]): three conditions for  $\hat{y}$ -component, five conditions for  $\hat{y}'$ -component, three conditions for  $y'$ -component, two conditions for  $y$ -component and four compatibility Conditions: we list the conditions in the tables below.

Table I

Order conditions for  $\hat{y}$

Order 2 Condition	$\sum_i \hat{b}_i = \frac{1}{2}$	(4.1)
Order 3 Condition	$\sum_i \hat{b}_i c_i = \frac{1}{6}$	(4.2)
Order 4 Condition	$\sum_i \hat{b}_i c_i^2 = \frac{1}{12}$	(4.3)

Table II

Order conditions for  $\hat{y}'$

Order 1 Condition	$\sum_i \hat{b}'_i = 1$	(4.4)
Order 2 Condition	$\sum_i \hat{b}'_i c_i = \frac{1}{2}$	(4.5)
Order 3 Condition	$\sum_i \hat{b}'_i c_i^2 = \frac{1}{3}$	(4.6)
Order 4 Condition 5	$\sum_i \hat{b}'_i c_i^2 = \frac{1}{4}$	(4.7)
	$\sum_{i,j}^i \hat{b}'_i a_{ij} c_j = \frac{1}{24}$	(4.8)

Table III

Order conditions for  $y$

Order 2 Condition	$\sum_i b_i = \frac{1}{2}$	(4.9)
Order 3 Condition	$\sum_i b_i c_i = \frac{1}{6}$	(4.10)

Table IV

Order condition for  $y'$

Order 1 Condition	$\sum_i b'_i = 1$	(4.11)
Order 2 Condition	$\sum_i b'_i c_i = \frac{1}{2}$	(4.12)
Order 3 Condition	$\sum_i b_i c_i = \frac{1}{3}$	(4.13)

The compapitibility conditions are given by

$$\frac{1}{2}c_j^2 = \sum_{k=1}^s a_{jk}, \quad (j= 1, 2, 3, 4) \tag{4.14}$$

To simplify the analysis, we use the following result due to [8].

$$\text{Let } b_j = b'_j(1 - c_j), \quad j = 1, \Lambda, s \tag{4.15}$$

then the order condition for the  $y$ -component are subset of the order conditions for the  $y'$ -component. The Tableau of the method is of the for

Table (4.1): The Butcher Tableau of the 4(3) DIRKN method

$c_1$	$\lambda$			
$c_2$	$a_{21}$	$\lambda$		
$c_3$	$a_{31}$	$a_{32}$	$\lambda$	
$c_4$	$a_{41}$	$a_{42}$	$a_{43}$	$\lambda$
	$b_1$	$b_2$	$b_3$	$b_4$
	$b'_1$	$b'_2$	$b'_3$	$b'_4$
	$\hat{b}_1$	$\hat{b}_2$	$\hat{b}_3$	$\hat{b}_4$
	$\hat{b}'_1$	$\hat{b}'_2$	$\hat{b}'_3$	$\hat{b}'_4$

Applying the (4.15), we therefore have twelve equations to solve in nineteen unknowns. Thus, we have seven free parameters. Let  $c_1$ ,  $c_2$ ,  $c_3$ ,  $c_4$ ,  $a_{32}$ ,  $a_{42}$  and  $b_1'$  be the free parameters. We start by solving the order conditions for  $\hat{y}'$  and  $\hat{y}$ . From (4.4), (4.5), (4.6) and (4.7) we obtain

$$\begin{aligned}\hat{b}_1' &= -\frac{-3+4c_2+4c_3-6c_2c_3+4c_4-6c_2c_4-6c_3c_4+12c_2c_3c_4}{12(c_1-c_2)(c_1-c_3)(c_1-c_4)} \\ \hat{b}_2' &= -\frac{3-4c_1-4c_3+6c_1c_3-4c_4+6c_1c_4+6c_3c_4-12c_1c_3c_4}{12(c_1-c_2)(c_2-c_3)(c_2-c_4)} \\ \hat{b}_3' &= -\frac{-3+4c_1+4c_2-6c_1c_2+4c_4-6c_1c_4+6c_2c_4+12c_1c_2c_4}{12(c_1-c_3)(c_2-c_3)(c_3-c_4)} \\ \hat{b}_4' &= -\frac{3-4c_1-4c_2+6c_1c_2-4c_3+6c_1c_3+6c_2c_3-12c_1c_2c_3}{12(c_1-c_4)(c_2-c_4)(c_3-c_4)}\end{aligned}$$

We then substitute into (4.8) and solve for  $a_{43}$  as

$$\begin{aligned}a_{43} &= ((c_1-c_3)(c_2-c_3)2a_{42}(c_1-c_2)(-3+c_2(4-6c_3)+4c_3+2c_1(2-3c_3+c_2(-3+6c_3))) \\ &+ ((1-4c_1-6c_1^2+12c_1^3)(c_1-c_4)(-c_2+c_4)(-c_3+c_4))-2a_{32}(c_1-c_2)(c_1-c_4)(c_2-c_4) \\ &\frac{(-3+c_2(4-6c_4)+4c_2+2c_1(2-3c_4+c_2)(-3+6c_4))}{(2(c_1-c_3)^2(-c_2+c_3)(-3+c_2(4-6c_3)+4c_3+2c_1(2-3c_3+c_2(-3+6c_3))))}\end{aligned}$$

From (4.14) we obtain

$$\begin{aligned}a_{41} &= \frac{1}{2}(-2a_{42}-c_1^2+c_4^2-((c_1-c_3)(c_2-c_3)(2a_{42}(c_1-c_2)(-3+c_2)(4-6c_3)) \\ &+ 4c_3+2c_1(2-3c_3+c_2(-3+6c_3))))+(1-4c_1-6c_1^2+12c_1^3)(c_1-c_4)(-c_2+c_4) \\ &(-c_3+c_4)-2a_{32}(c_1-c_2)(c_1-c_4)(c_2-c_4)(c_2-c_4)(-3+c_2(4-6c_4)+ \\ &+ 4c_4+2c_1(2-3c_4+c_2(-3+6c_4)))) \\ &\frac{(c_1-c_3)^2(-c_2+c_3)(-3+c_2(4-6c_3)+4c_3+2c_1(2-3c_3+c_2(-3+6c_3))))}{(c_1-c_3)^2(-c_2+c_3)(-3+c_2(4-6c_3)+4c_3+2c_1(2-3c_3+c_2(-3+6c_3))))}\end{aligned}$$

Again using (4.15) we obtain

$$\hat{b}_1 = -\frac{(1-c_1)(-3+4c_2+4c_3-6c_2c_3+4c_4-6c_2c_4-6c_3c_4+12c_2c_3c_4)}{12(c_1-c_2)(c_1-c_3)(c_1-c_4)}$$

$$\hat{b}_2 = -\frac{(1-c_2)(-3+4c_1+4c_3+6c_1c_3-4c_4+6c_1c_4+6c_3c_4-12c_1c_3c_4)}{12(c_1-c_2)(c_2-c_3)(c_2-c_4)}$$

$$\hat{b}_3 = -\frac{(1-c_3)(-3+4c_1+4c_2-6c_1c_2+4c_4+6c_1c_4-6c_2c_4-12c_1c_2c_4)}{12(c_1-c_3)(c_2-c_3)(c_3-c_4)}$$

$$\hat{b}_4 = -\frac{(1-c_4)(3+4c_1+4c_2-6c_1c_2-4c_3+6c_1c_3-6c_2c_3-12c_1c_2c_3)}{12(c_1-c_4)(c_2-c_4)(c_3-c_4)}$$

We now solve the order conditions for  $y'$  and  $y$ . Thus from (4.11), (4.12) and (4.13) we obtain

$$b'_2 = \frac{2-6b'_1c_1^2+c_4(-3+6b'_1c_1)+c_3(-3-6c_4(-1+b'_1)+6b'_1c_1)}{6(c_2-c_3)(c_2-c_4)}$$

$$b'_3 = \frac{-2+6b'_1c_1^2+c_4(3-6b'_1c_1)+c_2(3+6c_4(-1+b'_1)-6b'_1c_1)}{6(c_2-c_3)(c_3-c_4)}$$

$$b'_4 = \frac{2-6b'_1c_1^2+c_3(-3+6b'_1c_1)+c_2(-3-6c_3(-1+b'_1)+6b'_1c_1)}{6(c_2-c_4)(c_3-c_4)}$$

Also (4.15), we obtain  $b_1 = (1-c_1)b'_1$

$$b_2 = \frac{(-1+c_2)(-2+6b'_1c_1^2+c_4(3-6b'_1c_1)+c_3(3+6c_4)(-1+b'_1)-6b'_1c_1)}{6(c_2-c_3)(c_2-c_4)}$$

$$b_3 = \frac{(-1+c_3)(-2+6b'_1c_1^2+c_4(3-6b'_1c_1)+c_2(3+6c_4)(-1+b'_1)-6b'_1c_1)}{6(c_2-c_3)(c_3-c_4)}$$

$$b_4 = \frac{(-1+c_4)(-2+6b'_1c_1^2+c_3(3-6b'_1c_1)+c_2(3+6c_3)(-1+b'_1)-6b'_1c_1)}{6(c_2-c_4)(c_3-c_4)}$$

The principal truncation error coefficients of the higher order method are given by

$$\hat{T}'_{41} = \hat{T}'_{42} = \hat{T}'_{43} = \sum_i b_i = c_i^4 - \frac{1}{5} ; \quad \hat{T}'_{44} = \sum_{i,j} b_i c_i a_{ij} c_j - \frac{4}{120}$$

$$\hat{T}'_{45} = \hat{T}'_{46} = \sum_{i,j} b_i a_{ij} c_j^2 - \frac{1}{60} ; \quad \hat{T}'_{41} = \hat{T}'_{42} = \sum_i b_i c_i^3 - \frac{1}{4}$$

(4.16)



We minimize the principal truncation error coefficients with respect to  $c_1, c_2, c_3, c_4, a_{32}, a_{42}$  and  $b_1'$  to obtain values for the free parameters. The choice of  $c_1 = \frac{1}{10}, c_2 = \frac{1}{5}, c_3 = \frac{6}{25}, c_4 = \frac{4}{5}, a_{32} = -\frac{1}{2}, a_{42} = \frac{7}{10}$  and  $b_1' = -\frac{1}{25}$  gives the coefficients of the tableau (4.1) for the embedded DIRKN 4(3) method.

Table (4.2): The Butcher Tableau of the coefficients of the 4(3) DIRKN method

$\frac{1}{10}$	$\frac{1}{200}$			
$\frac{1}{5}$	$\frac{3}{200}$	$\frac{1}{200}$		
$\frac{6}{25}$	$\frac{2619}{5000}$	$-\frac{1}{2}$	$\frac{1}{200}$	
$\frac{4}{5}$	$-\frac{170241}{194600}$	$\frac{7}{10}$	$\frac{2382}{4865}$	$\frac{1}{200}$
$\frac{1}{5}$	$-\frac{9}{250}$	$\frac{347}{1125}$	$\frac{551}{4200}$	$\frac{6071}{63000}$
	$-\frac{1}{25}$	$\frac{347}{900}$	$\frac{29}{168}$	$\frac{6071}{12600}$
	$\frac{39}{245}$	$-\frac{2}{5}$	$\frac{95}{145}$	$\frac{139}{1470}$
	$\frac{26}{147}$	$-\frac{1}{2}$	$\frac{125}{1471}$	$\frac{139}{294}$

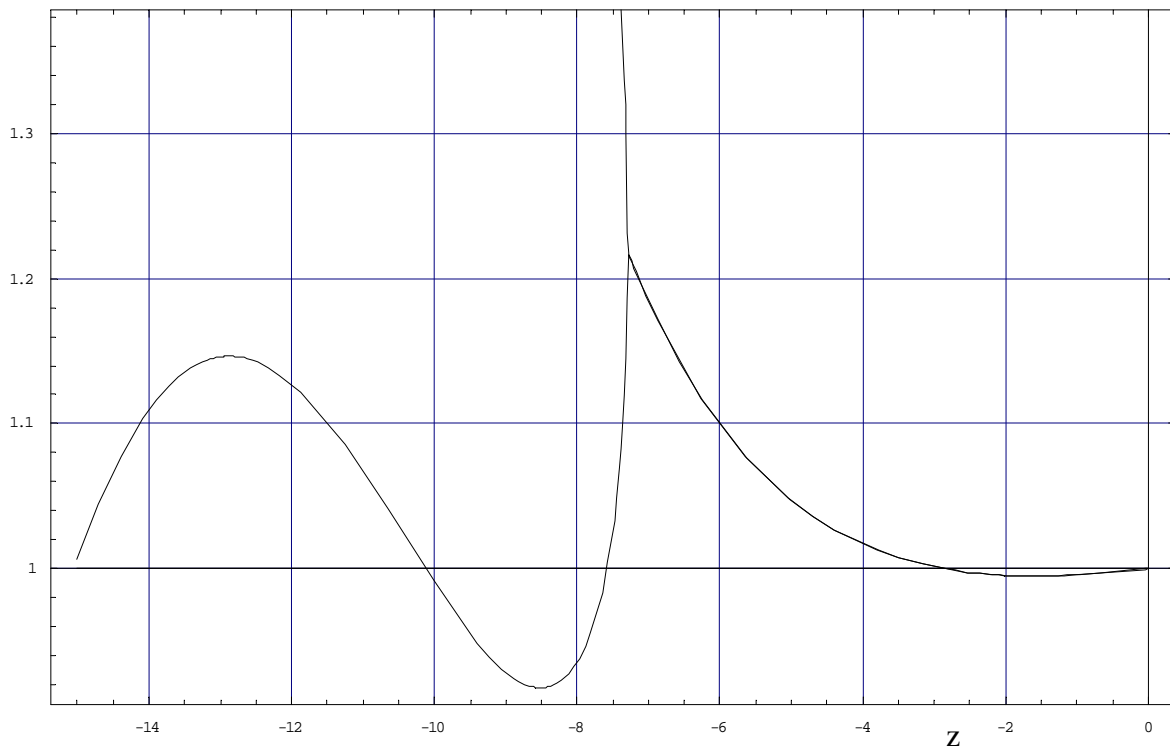
The local truncation error estimate for the method are given by

$$\begin{aligned} \Delta_{n+1} &= h^2 \left( -\frac{2391}{12250} F_1 + \frac{797}{1125} F_2 - \frac{15143}{29400} F_3 + \frac{797}{441000} F_4 \right) \\ \Delta'_{n+1} &= h \left( -\frac{797}{3675} F_1 + \frac{797}{900} F_2 + \frac{21659}{247128} F_3 + \frac{797}{88200} F_4 \right) \end{aligned} \quad (4.17)$$

We now examine the stability of the method. The amplification matrix is given by

$$R(z) = \begin{bmatrix} 1 + \frac{1}{2}z + \frac{26}{625}z^2 - \frac{3}{1250}z^3 - \frac{1}{2500}z^4 & 1 + \frac{833}{5000}z - \frac{29}{2000}z^2 - \frac{7}{2500}z^3 + \frac{1}{10000}z^4 \\ z + \frac{833}{5000}z^2 + \frac{57}{10000}z^3 - \frac{1}{625}z^4 & 1 + \frac{1}{2}z + \frac{26}{625}z^2 - \frac{27}{2500}z^3 - \frac{3}{10000}z^4 \end{bmatrix}$$

A plot of the roots of  $R(z)$  against  $z$  shows that the polynomial  $R_j(z)$ ,  $j = 1, 2, 3$  as defined by (3.5) are nonnegative if  $z \in (-3.2, 0)$ , yielding the stability boundary  $z_0 = 3.2$ , see the graph in fig.4.1 for the stability plot of  $|R(z)|$ . Hence the method is R-stable within the interval.



**Fig. (4.1): Absolute Root locus plot of  $|R(z)|$  versus  $z$**

## 5. Conclusion

[13] and [15] derived the implicit cases of the RKN methods, but are not embedded. In fact, there has not been much work on embedded implicit methods so far arising from the difficulties of deriving its coefficients and its implementation when compared to the explicit case of the class of the method. In this paper, we

have developed a class of four-stage embedded DIRKN method of orders 4(3) for the numerical solution of the initial value problem of the special second order differential equation (1.1) possessing oscillatory solution. The scheme controls the local error in the solution and the derivative. The error estimate is obtained by using an

embedded method. The embedded formula, see table (4.2) for the DIRKN method have been chosen so that its stability matrix has bounded eigen-values and R-stable, thus suitable for oscillatory problems. Also, for the method in table (4.2) derived, the minimization of the principal truncation error coefficients (4.16) leads to the minimized local truncation error in (4.17) used for variable step-size implementation of the method in table (4.2).

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