Development and Investigation of Runge-Kutta Coefficients Dependent Stability Polynomial

Salau T.A.O.
Department of Mechanical Engineering
University of Ibadan
Ibadan, Nigeria
tao.salau@mail.ui.edu.ng

Ajide O.O.
Department of Mechanical Engineering
University of Ibadan
Ibadan, Nigeria
ooe.ajide@mail.ui.edu.ng

Abstract—Simulation of reliable solutions of nonlinear engineering problems by means of stable numerical algorithms is a frequent and acceptable practice. This study focuses the development and investigation of Runge-Kutta coefficients dependent stability polynomial for the second, third and fourth orders Runge-Kutta schemes. The development utilized matrix inversion operation procedure that involves determinant and cofactors computation of relevant matrix. The validation was made referencing the standard result of [1] and extended to several cases. The resulting polynomials obtained consist of combination of the scheme coefficients with increasing power of time step that follows a rhyme pattern. The validation test case result agreed perfectly with test standard result. Selected studied version of different schemes shows wide variation in the shape of stability curve and region bounded. It is interesting to note that the popular second, third and fourth order schemes have stability curve that bounded larger region than their respective counterpart. It is concluded that the study results can be utilized as reliable platform for stability analysis for different versions of the second, third and fourth order schemes.

Keywords- Runge-Kutta Coefficients; Polynomial; Time step; Matrix Inversion and Stability Curve

I. INTRODUCTION

[2] described polynomial as an expression that have constants, variables and exponents (but: no division by a variable; it cannot have an infinite number of terms and a variable exponents that can only be 0, 1, 2, 3, ------ e.t.c). [3] defined polynomial as an algebraic expression consisting of a constant multiplication and one or more variables raise to an integral power. The relevance of polynomial equation in sciences and engineering cannot be overemphasized. Polynomial equation has been used as the foundation for numerous numerical modelling in engineering. Significant research efforts have been made in the adoption of polynomials in nonlinear dynamics. Generalized polynomial chaos has been identified to fail for long term integration. This is because it experienced a continuous deterioration in its optimal convergence behaviour which in turn leads to very high error-levels. [4] studied a time-dependent alternative of polynomial chaos in order to overcome the problem of deterioration in behaviour. The author reinitialized the polynomial chaos expansion of the solution discretely in time based on the statistics of the evolved solution at this discrete time-level. This allows a low order polynomial expansion at each instant in order to attain satisfactory precisions. The author's finding has demonstrated that the time-dependent polynomial chaos is capable of solving a one-dimensional stochastic ordinary differential equation. A multi-element generalized polynomial chaos method for arbitrary probability measures has been developed by [5]. This method was applied to solve ordinary and partial differential equations with stochastic inputs. Numerical experiments revealed that the cost for the construction of orthogonal polynomial is negligible compared to the total computation time cost. This finding has again reinforced the nonlinearity characteristics of polynomial dynamics. [6] paper presented a new Lauerre's type method for solving of polynomial equations with real coefficients. The paper extensively demonstrated the effectiveness of the method for solving many practical problems. A study which provides a proof of a relationship theorem between nonlinear analogue polynomial equations and the corresponding Jacobian matrix has been studied by [7] .This theorem has been satisfied to be effective for all nonlinear polynomial algebraic system equations. The presented theorem has a benefit of reducing numerical catalogue equations of nonlinear initial value problems to the simple linear ones without any linearization procedures. [8] paper focused on computing stability regions Runge-Kutta methods for delay differential equations. Practical determination of stability regions when various

fixed-step wise Runge-Kutta methods combined with continuous extensions are applied to the linear differential equation with fixed delay parameter. The paper extensively explained an alternative stability boundary algorithm that overcomes the difficulties encountered using the boundary locus technique. This new algorithm is applicable for both explicit and implicit Runge-Kutta methods. [9] studied the flexible stability domains for explicit Runge-Kutta methods. The paper presented families of stability polynomials for explicit Runge-Kutta methods that exhibit some optimality. These families were employed to construct Runge-Kutta methods that adaptively follow a spectrum given in a respective application without the need of reducing the time step. The optimal stability polynomials for explicit Runge-Kutta were specifically applied for advection-diffusion dynamics. Findings show that for strong diffusion of fine grids, more stages are employed in order to maintain a time step controlled by the Advection alone. Strong stability high order Runge-Kutta time discretizations were developed by [10] for application with semi-discrete method of lines approximations of hyperbolic partial differential equations. In their paper, an optimal strong stability preserving Runge-Kutta methods as well as a bound on the optimal time step restriction was studied. The authors concluded that the development of strong stability preserving Runge-Kutta methods was primarily geared toward linear operations and the wide applicability of these methods. The problem of fault detection and isolation has been applied by [11] for nonlinear systems that are modelled by polynomial differentiation algebraic equations. The authors adopted Ritt's algorithm in obtaining an input-output representation of the monitored system by eliminating unknown variables. The simulation results obtained demonstrated the importance of fault detection and isolation in modelling nonlinear systems that are modelled by polynomial equations. Methods for detecting and localizing time singularities of polynomial and quasi-polynomial ordinary differential equation has been studied and developed by [12]. The authors satisfactorily adopted these methods in several fields of system dynamics. This includes systems such as decoupling, Lotka Voltera form, companion system and global lipschitz property.

From the foregoing, there is no doubt that an extensive work has been made in the applications of polynomials in the study of nonlinear dynamics. Notwithstanding this landmark research output in this field, vigorous efforts are yet to be made in the development as well as the investigation of Runge-Kutta coefficients dependent stability polynomial. This research dearth strongly motivates the present paper. The aim of this research paper is to develop and investigate the dynamics of dependent stability polynomial for the second, third and fourth orders Runge-Kutta schemes.

II. METHODOLOGY

[13] refers, the numerical method of Runge-Kutta is devoted to solving ordinary differential equations of the general form given by equation (1). However, the step by step numerical solution of equation (1) is given by equation (2), with ϕ being an incremental weighting function. The general form for ϕ is given by equation (3). According to equation (3), the slope estimate of ϕ is used to extrapolate from an old value y_i to a new value y_{i+1} over a step size h.

$$\frac{dy}{dx} = f(x,y) \tag{1}$$

$$y_{i+1} = y_i + \phi h \tag{2}$$

$$\phi = c_1 K_1 + c_2 K_2 + \bullet\bullet\bullet + c_n K_n \tag{3}$$

The functions K_1 to K_2, K_1 to K_3 and K_1 to K_4 for the respective second, third and fourth order Runge-Kutta schemes are given by equations (4) to (5), equations (4) to (6) and equations (4) to (7). The equivalents of equation (2) for the second, third and fourth schemes are given respectively by equations (8), (9) and (10).

$$K_1 = f(x_i, y_i) \tag{4}$$

$$K_2 = f(x_i + a_2 h, y_i + b_{21} K_1) \tag{5}$$

$$K_3 = f(x_i + a_3 h, y_i + b_{31} K_1 + b_{32} K_2) \tag{6}$$

$$K_4 = f(x_i + a_4 h, y_i + b_{41} K_1 + b_{42} K_2 + b_{43} K_3) \tag{7}$$

$$y_{i+1} = y_i + h\left\{c_1 K_1 + c_2 K_2\right\} \tag{8}$$

$$y_{i+1} = y_i + h\left\{c_1 K_1 + c_2 K_2 + c_3 K_3\right\} \tag{9}$$

$$y_{i+1} = y_i + h\left\{c_1 K_1 + c_2 K_2 + c_3 K_3 + c_4 K_4\right\} \tag{10}$$

[1] and [14] provided detail coefficients algebraic relationship and simulation presented in graphics. The two studies adopted the equivalent relationship with the corresponding coefficients in Taylor series expansion of the function $f(x, y)$ to the nth–order terms that was supplemented by Butcher simplifying assumption implied by equation (11).

$$\sum_{i=1}^{s} c_i b_{ij} = c_j(1-a_j),\ j = 2,3,4 \tag{11}$$

[3] defined the stability polynomial (R*(h)*) in the general term as equation (12) for time step size (h) and c^T, A and e given by equations (13) to (16), equations (17) to (20) and equations (21) to (24) for the second, third and fourth order scheme respectively. It is required that $|R(h)| < 1$ for absolute stability. However, the stability curve outlines in the present study were defined as $0.99 \le |R(h)| \le 1.00$ and evaluated at constant length step size of 0.01 on the plane with real and imaginary lengths defined respectively as $-3.00 \le \mathrm{Re}(h) \le 1.00$ and $-3.00 \le \mathrm{Im}(h) \le 1.00$

$$R(h) = 1 + hc^T (I - hA)^{-1} e = 1 + hc^T B^{-1} e \tag{12}$$

A. Runge-Kutta Second Order scheme

$$c^T = \{c_1 \quad c_2\} \tag{13}$$

$$A = \begin{bmatrix} 0 & 0 \\ b_{21} & 0 \end{bmatrix} \tag{14}$$

$$I - hA = B = \begin{bmatrix} 1 & 0 \\ -hb_{21} & 1 \end{bmatrix} \tag{15}$$

$$e = \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \tag{16}$$

B. Runge-Kutta Third Order scheme

$$c^T = \{c_1 \quad c_2 \quad c_3\} \tag{17}$$

$$A = \begin{bmatrix} 0 & 0 & 0 \\ b_{21} & 0 & 0 \\ b_{31} & b_{32} & 0 \end{bmatrix} \tag{18}$$

$$I - hA = B = \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 1 & 0 \\ -hb_{31} & -hb_{32} & 1 \end{bmatrix} \tag{19}$$

$$e = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} \tag{20}$$

C. Runge-Kutta Fourth Order scheme

$$c^T = \{c_1 \quad c_2 \quad c_3 \quad c_4\} \tag{21}$$

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ b_{21} & 0 & 0 & 0 \\ b_{31} & b_{32} & 0 & 0 \\ b_{41} & b_{42} & b_{43} & 0 \end{bmatrix} \tag{22}$$

$$I - hA = B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -hb_{21} & 1 & 0 & 0 \\ -hb_{31} & -hb_{32} & 1 & 0 \\ -hb_{41} & -hb_{42} & -hb_{43} & 1 \end{bmatrix} \tag{23}$$

$$e = \begin{Bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{Bmatrix} \tag{24}$$

The inverse of arbitrary matrix and that of matrix (B) depends on its determinant and cofactors matrix (F) as in equation (25).

$$B^{-1} = \frac{(F)^T}{\det B} \tag{25}$$

The determinant of matrix (B) for the three schemes is same and is given by equation (26).

$$\det B = 1 \tag{26}$$

D. Coefficients of Validation Case

The under listed coefficients adopted from [1] for the fourth order scheme were used to validate this study.

$$c^T = \begin{Bmatrix} \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} \end{Bmatrix}; \; b_{21} = \frac{1}{3}; \; b_{31} = -\frac{1}{3}; \; b_{32} = 1; \; b_{41} = 1; \; b_{42} = -1; \; b_{43} = 1.$$

III. RESULTS AND DISCUSSIONS

In this study, focus is on the fourth order scheme with extension of results applied to the second and third order schemes. Therefore, the relative details of computation of the sixteen entries of the cofactors matrix for the fourth scheme are under listed.

$$F_{11} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{32} & 1 & 0 \\ -hb_{42} & -hb_{43} & 1 \end{bmatrix} \right\| = 1$$

$$F_{12} = -1 \times \left\| \begin{bmatrix} -hb_{21} & 0 & 0 \\ -hb_{31} & 1 & 0 \\ -hb_{41} & -hb_{43} & 1 \end{bmatrix} \right\| = hb_{21}$$

$$F_{13} = \left\| \begin{bmatrix} -hb_{21} & 1 & 0 \\ -hb_{31} & -hb_{32} & 0 \\ -hb_{41} & -hb_{42} & 1 \end{bmatrix} \right\| = b_{21}b_{32}h^2 + b_{31}h$$

$$F_{14} = -1 \times \left\| \begin{bmatrix} -hb_{21} & 1 & 0 \\ -hb_{31} & -hb_{32} & 1 \\ -hb_{41} & -hb_{42} & -hb3 \end{bmatrix} \right\| = b_{21}b_{32}b_{43}h^3 + (b_{21}b_{42} + b_{31}b_{43})h^2 + b_{41}h$$

$$F_{21} = -1 \times \left\| \begin{bmatrix} 0 & 0 & 0 \\ -hb_{32} & 1 & 0 \\ -hb_{42} & -hb_{43} & 1 \end{bmatrix} \right\| = 0$$

$$F_{22} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{31} & 1 & 0 \\ -hb_{41} & -hb_{43} & 1 \end{bmatrix} \right\| = 1$$

$$F_{23} = -1 \times \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{31} & -hb_{32} & 0 \\ -hb_{41} & -hb_{42} & 1 \end{bmatrix} \right\| = b_{32}h$$

$$F_{24} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{31} & -hb_{32} & 1 \\ -hb_{41} & -hb_{42} & -hb_{43} \end{bmatrix} \right\| = b_{32}b_{43}h^2 + b_{42}h$$

$$F_{31} = \left\| \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -hb_{42} & -hb_{43} & 1 \end{bmatrix} \right\| = 0$$

$$F_{32} = -1 \times \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 0 & 0 \\ -hb_{41} & -hb_{43} & 1 \end{bmatrix} \right\| = 0$$

$$F_{33} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 1 & 0 \\ -hb_{41} & -hb_{42} & 1 \end{bmatrix} \right\| = 1$$

$$F_{34} = -1 \times \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 1 & 0 \\ -hb_{41} & -hb_{42} & -hb_{43} \end{bmatrix} \right\| = b_{43}h$$

$$F_{41} = -1 \times \left\| \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ -hb_{32} & 1 & 0 \end{bmatrix} \right\| = 0$$

$$F_{42} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 0 & 0 \\ -hb_{31} & 1 & 0 \end{bmatrix} \right\| = 0$$

$$F_{43} = -1 \times \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 1 & 0 \\ -hb_{31} & -hb_{32} & 0 \end{bmatrix} \right\| = 0$$

$$F_{44} = \left\| \begin{bmatrix} 1 & 0 & 0 \\ -hb_{21} & 1 & 0 \\ -hb_{31} & -hb_{32} & 1 \end{bmatrix} \right\| = 1$$

$$F^T = \begin{bmatrix} F_{11} & F_{21} & F_{31} & F_{41} \\ F_{12} & F_{22} & F_{32} & F_{42} \\ F_{13} & F_{23} & F_{33} & F_{43} \\ F_{14} & F_{24} & F_{34} & F_{44} \end{bmatrix} \tag{27}$$

Use equations (26) and (27) in equation (25) to obtain the inverse of matrix (B). Thereafter, use the inverse of matrix (B), equations (21) and (24) in equation (12) to obtain the Runge-Kutta coefficients dependent stability polynomial for the fourth order scheme given by equation (28).

$$R(h) = 1.0 + (c_1 + c_2 + c_3 + c_4)h + \left\{c_2 b_{21} + c_3(b_{31} + b_{32}) + c_4(b_{41} + b_{42} + b_{43})\right\} h^2 + \left\{c_3 b_{21} b_{32} + c_4(b_{21} b_{42} + b_{21} b_{31} + b_{32} b_{43})\right\} h^3 + c_4 b_{21} b_{32} b_{43} h^4$$
(28)

Furthermore, the corresponding form of equation (28) can be obtained for the third order scheme by first repeating the procedure for the cofactors computation for matrix (B) given by equation (19). Thereafter use the inverse of matrix (B) obtained in conjunction with equations (17) and (20) in equation (12) to obtain the stability polynomial for the third order scheme expressed in term of the Runge-Kutta coefficients given by equation (29).

$$R(h) = 1.0 + (c_1 + c_2 + c_3)h + \left\{c_2 b_{21} + c_3(b_{31} + b_{32})\right\} h^2 + c_3 b_{21} b_{32} h^3 \tag{29}$$

Similarly, the stability polynomial for the second order scheme expressed in term of the relevant Runge-Kutta coefficients is by extension of procedure given by equation (30).

$$R(h) = 1.0 + (c_1 + c_2)h + c_2 b_{21} h^2 \tag{30}$$

Equations (28), (29) and (30) refer, consistent and discernable pattern can be observed between the coefficients combination and increasing power of time step (h). In addition, the stability polynomial result given by equation (31) is obtained when the coefficients of the validation case are inserted into equation (28). This polynomial agreed perfectly with that of [1] or the popular version of fourth order Runge-Kutta scheme.

$$R(h) = 1.0 + h + \frac{1}{2}h^2 + \frac{1}{6}h^3 + \frac{1}{24}h^4 \tag{31}$$

Table 1: Coefficients of Selected Version of Fourth Order Scheme

Cases	b_{21}	b_{31}	b_{32}	b_{41}	b_{42}	b_{42}	c_1	c_2	c_3	c_4
RK41	0.500	0.000	0.500	0.000	0.000	1.000	0.167	0.333	0.333	0.167
RK42	0.333	-0.339	1.007	1.013	-1.011	0.998	0.878	-0.377	0.374	0.124
RK43	0.775	0.380	0.152	-0.088	-0.736	1.824	-0.076	0.125	0.757	0.194
RK44	0.518	-0.613	1.039	-0.184	0.715	0.469	1.236	-0.536	0.135	0.165
RK45	0.741	0.547	0.092	0.459	-1.614	2.155	-2.161	1.176	1.700	0.285

Table 2: Coefficients of Selected Fourth Order Scheme Stability Polynomial

Cases	$c_4 b_{21} b_{32} b_{43}$	$c_3 b_{21} b_{32} + c_4(b_{21} b_{42} + b_{21} b_{31} + b_{32} b_{43}$	$c_2 b_{21} + c_3(b_{31} + b_{32}) + c_4(b_{41} + b_{42} + b_{43}$	$\sum_{i=1}^{i=4} c_i$
RK41	0.042	0.167	0.500	1.000
RK42	0.042	0.195	0.249	1.000
RK43	0.042	0.089	0.694	1.000
RK44	0.042	0.162	-0.055	1.000
RK45	0.042	-0.054	2.242	1.000

Table 3: Coefficients of Selected Version of Third Order Scheme

Cases	b_{21}	b_{31}	b_{32}	c_1	c_2	c_3
RK31	0.500	-1.000	2.000	0.167	0.667	0.167
RK32	0.333	0.444	0.224	-1.246	0.011	2.235
RK33	0.775	0.134	0.398	-0.213	0.673	0.540
RK34	0.518	0.514	-0.089	-1.266	5.897	-3.631
RK35	0.741	0.345	0.294	-0.057	0.291	0.766

Table 4: Coefficients of Selected Third Order Scheme Stability Polynomial

Cases	$c_3 b_{21} b_{32}$	$c_2 b_{21} + c_3(b_{31} + b_{32})$	$\sum_{i=1}^{i=3} c_i$
RK31	0.167	0.500	1.000
RK32	0.167	1.497	1.000
RK33	0.167	0.809	1.000
RK34	0.167	1.511	1.000
RK35	0.167	0.705	1.000

Table 5: Coefficients of Selected Version/Stability Polynomial of Second Order Scheme

Cases	b_{21}	c_1	c_2	$c_2 b_{21}$	$\sum_{i=1}^{i=2} c_i$
RK21	1.000	0.500	0.500	0.500	1.000
RK22	5.000	0.100	0.900	4.500	1.000
RK23	2.500	0.200	0.800	2.000	1.000
RK24	1.670	0.300	0.700	1.169	1.000
RK25	1.250	0.400	0.600	0.750	1.000

Tables 1 to 5 contain in detail the coefficients of selected samples of version and stability polynomial for second, third and fourth order Runge-Kutta schemes. It is worth noting that RK21, RK31 and RK41 refer respectively to the popular second, third and fourth order version of Runge-Kutta schemes. It is observed that the stability polynomial vary in details for studied cases and schemes. The selected samples of stability curve outline are given in figures 1 to 9.

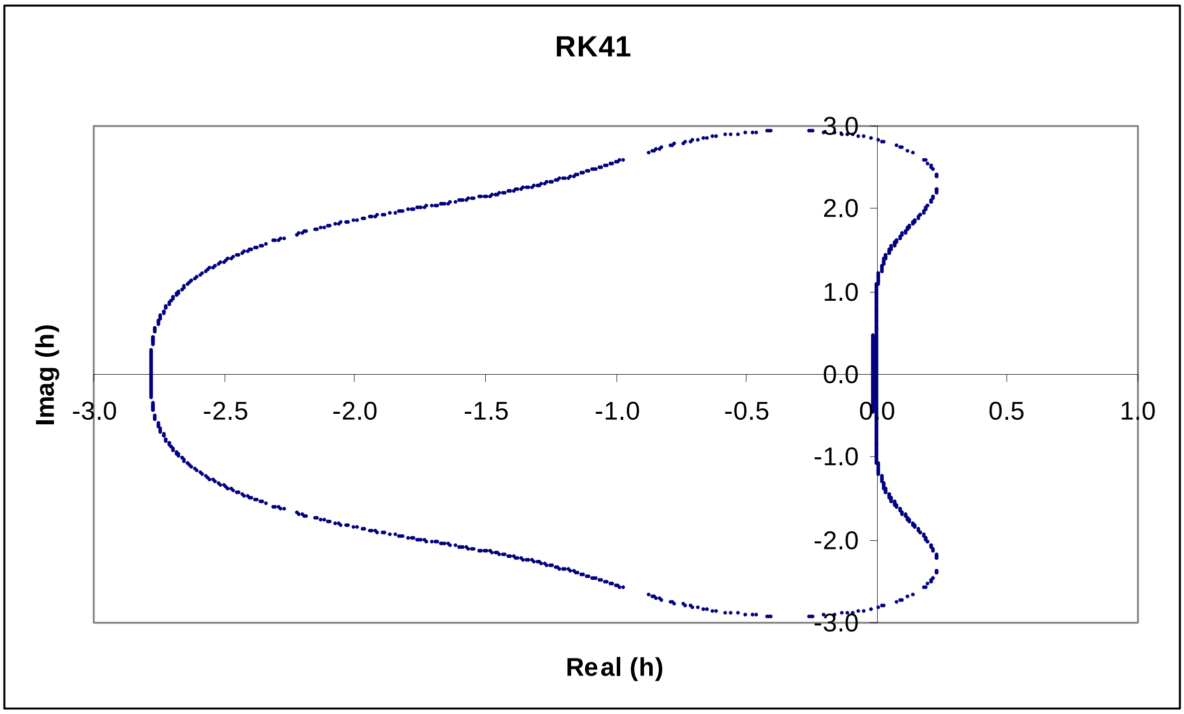

Figure 1: Stability polynomial scatter plot for RK41.

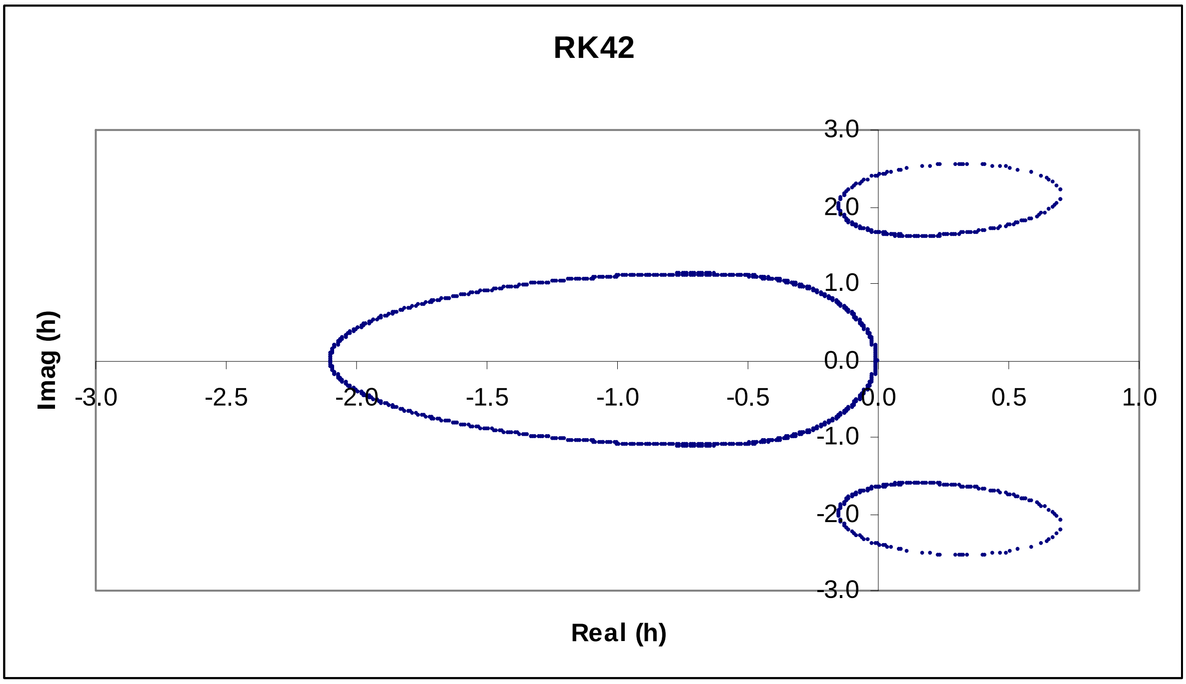

Figure 2: Stability polynomial scatter plot for RK42

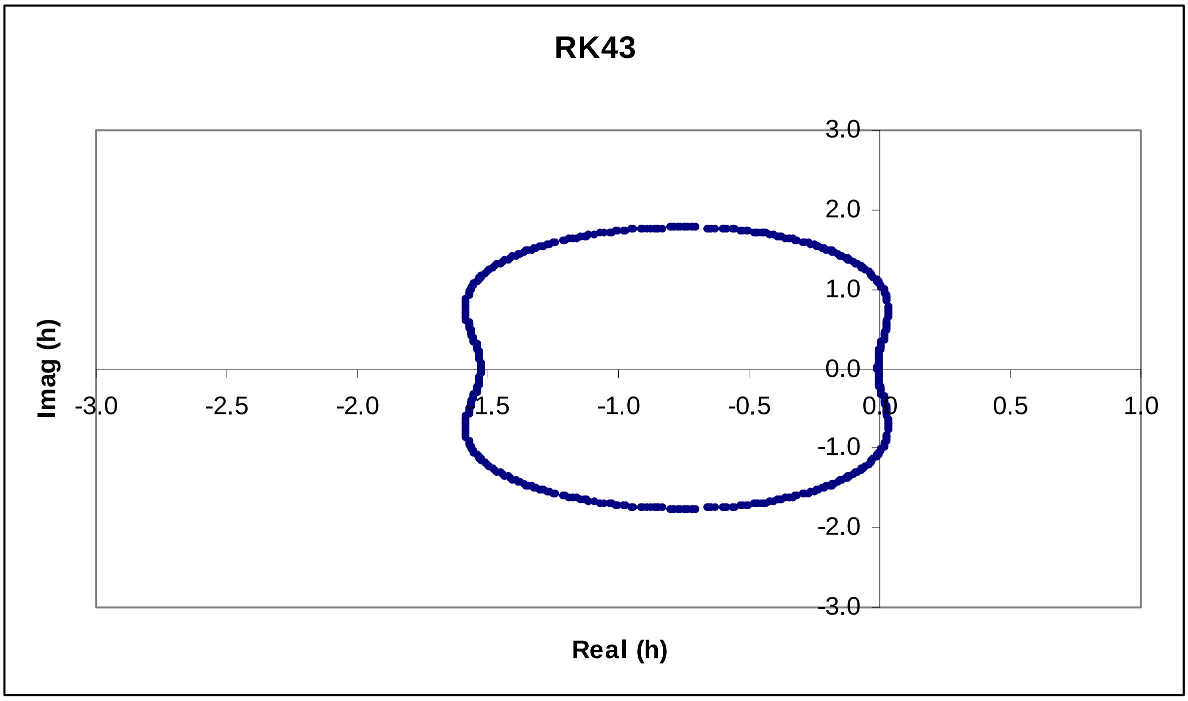

Figure 3: Stability polynomial scatter plot for RK43

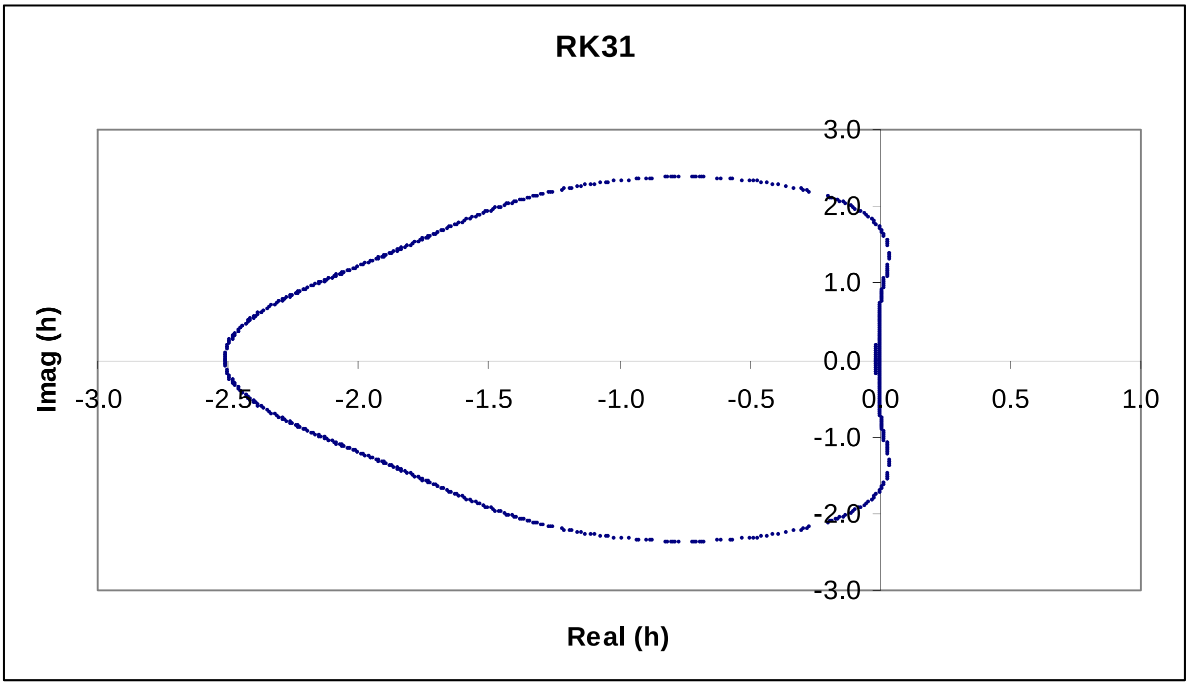

Figure 4: Stability polynomial scatter plot for RK31

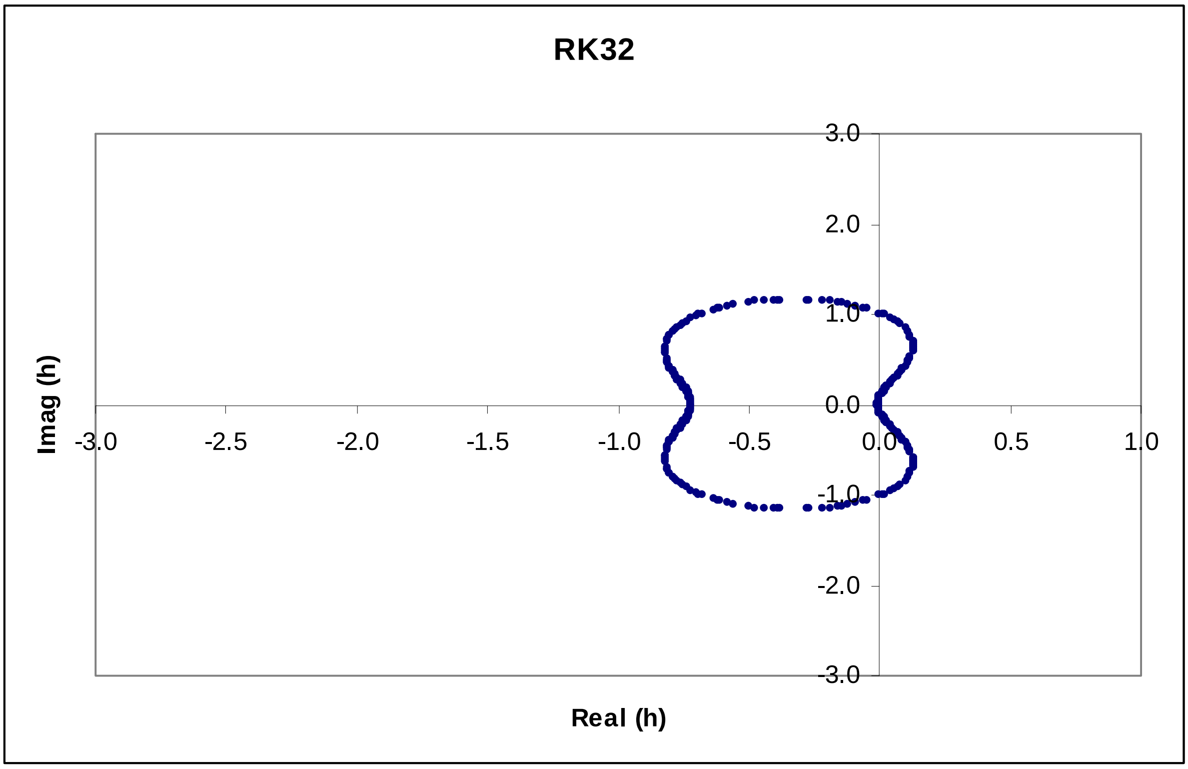

Figure 5: Stability polynomial scatter plot for RK32

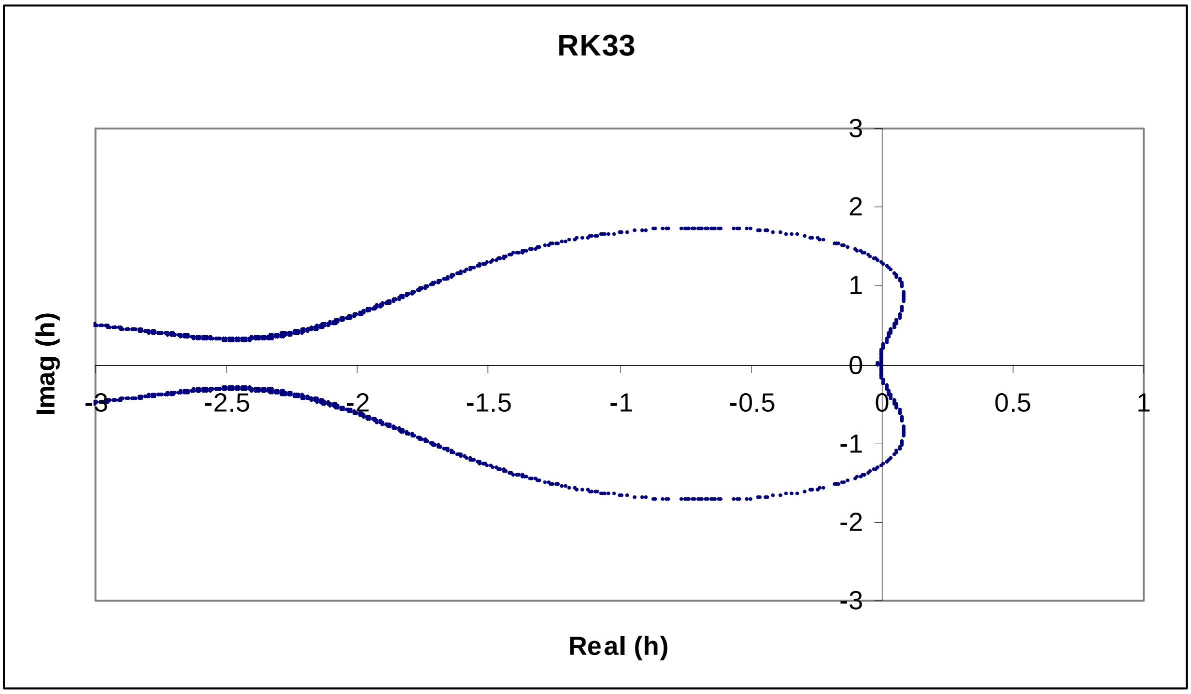

Figure 6: Stability polynomial scatter plot for RK33

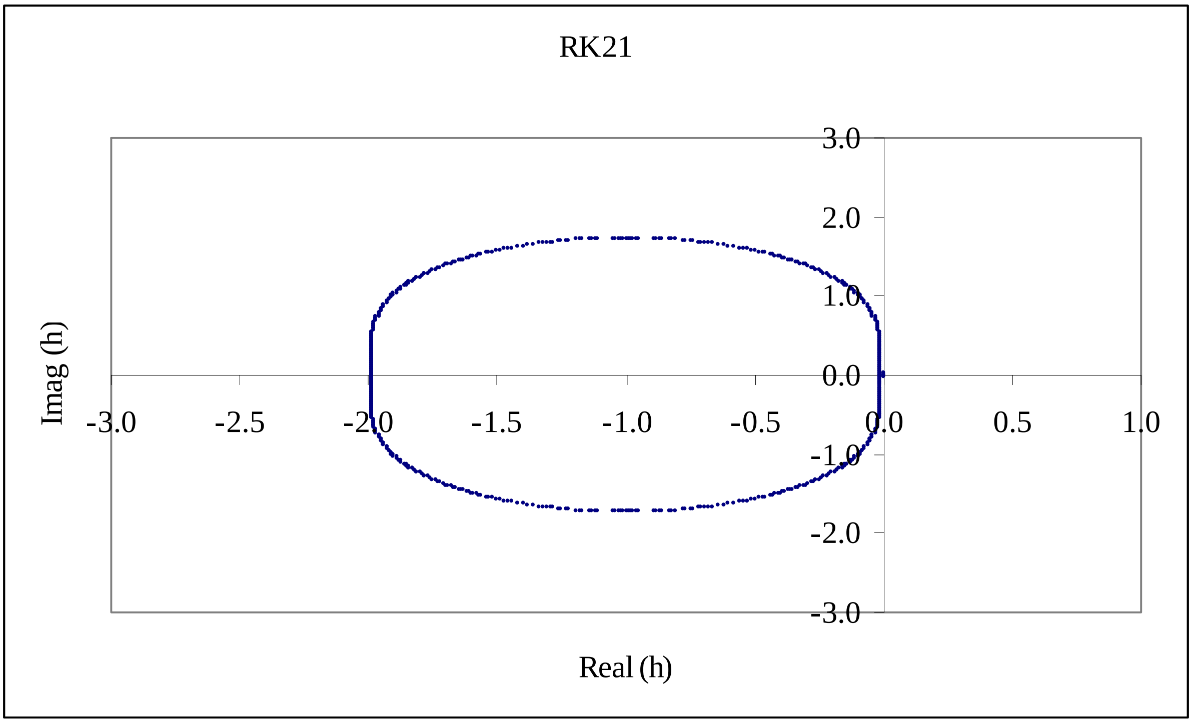

Figure 7: Stability polynomial scatter plot for RK21

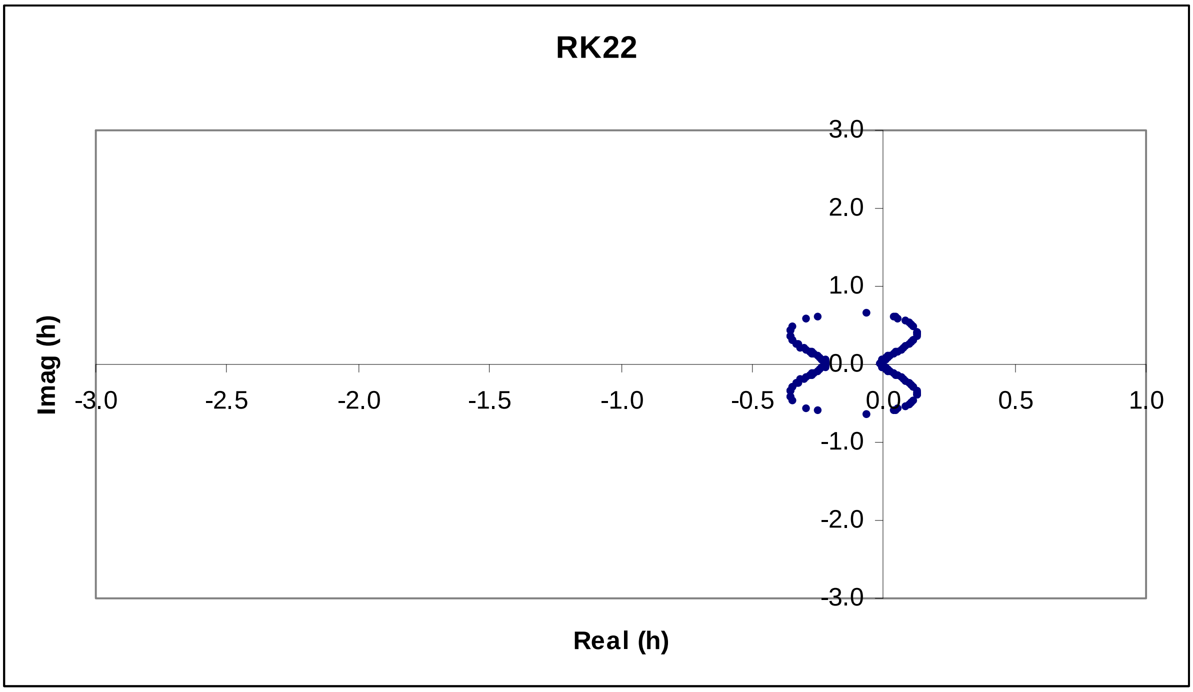

Figure 8: Stability polynomial scatter plot for RK22

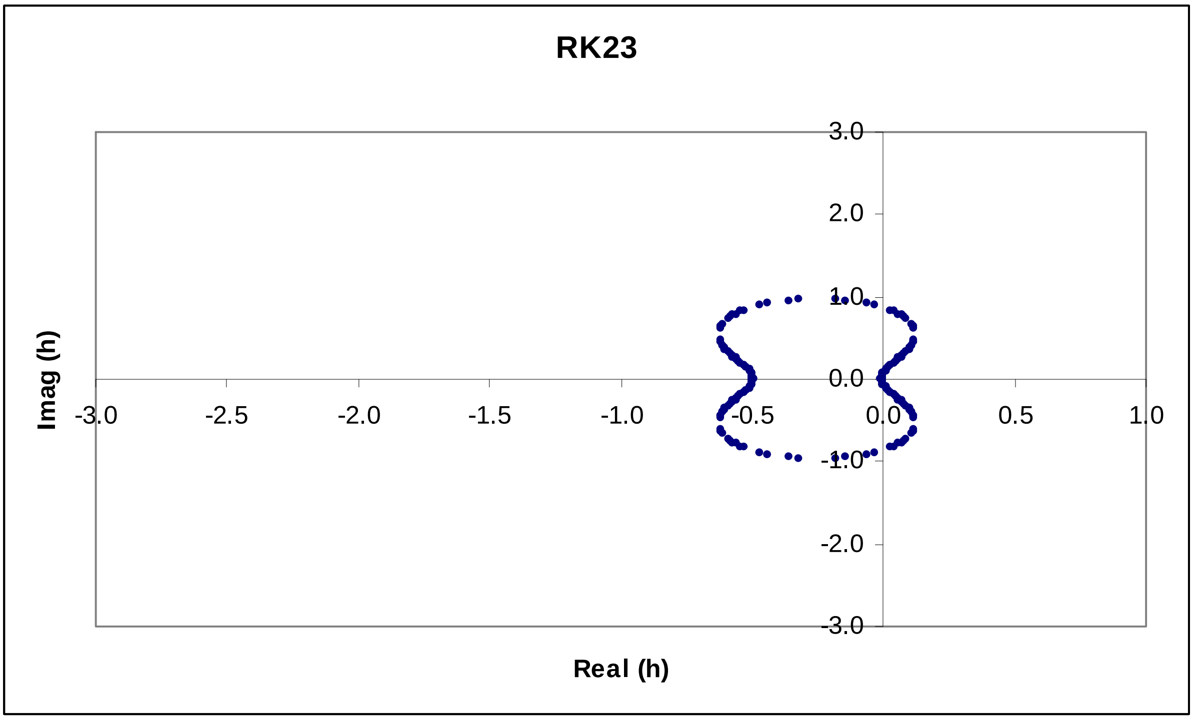

Figure 9: Stability polynomial scatter plot for RK23

Referring to figures 1 to 9, visual assessment shows that the stability curves vary in shape and quantity of bounded region over studied cases. The stability curve of RK42 comprises of three disjointed pieces with a total bounded region area smaller than the corresponding RK41. Furthermore, the stability curve of the popular second, third and fourth order schemes bounded more region than other corresponding studied cases. This observation on large bounded stable region is one of the factors for their popularity. The stability curve of RK43 and RK32 resemble qualitatively and likewise RK22 and RK23. However the bounded stable region of RK43 is higher than that of RK32. RK22 is the poorest measured in term of lowest bounded stable region area among figures 1 to 9. The curve of RK33 is not closed at the left end of the real axis.

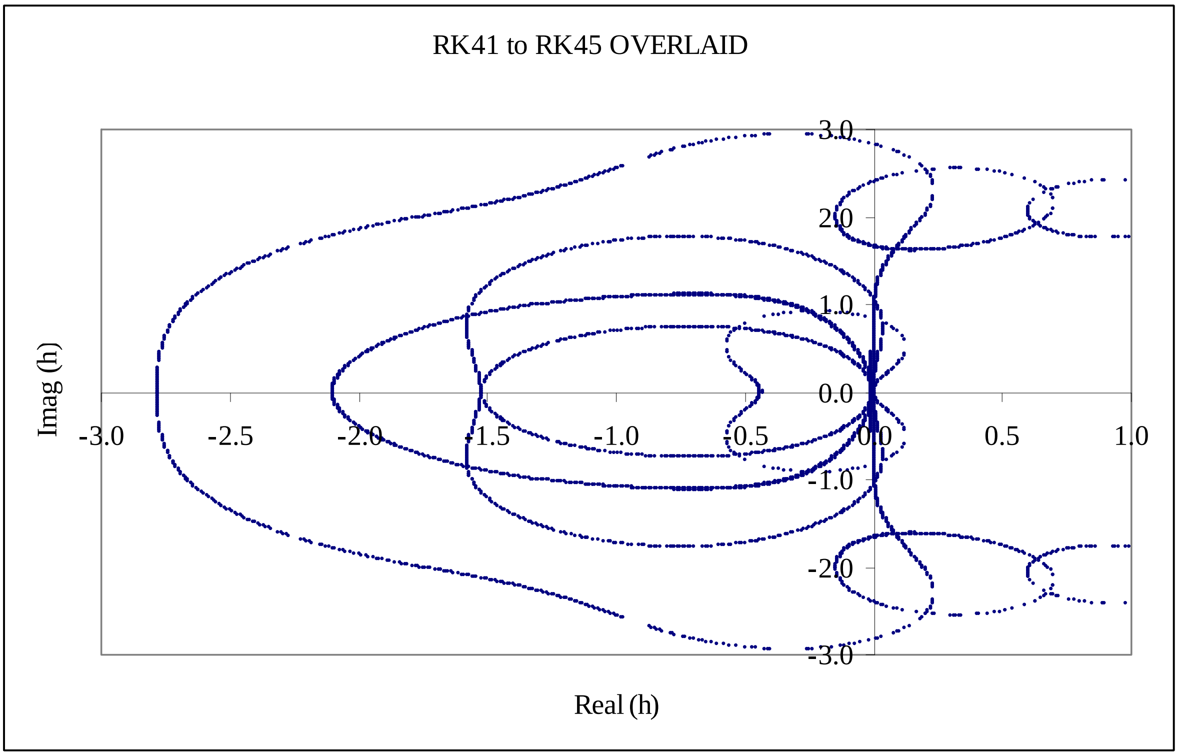

Figure 10: Overlaid stability curves for the fourth order scheme (RK41 to RK45)

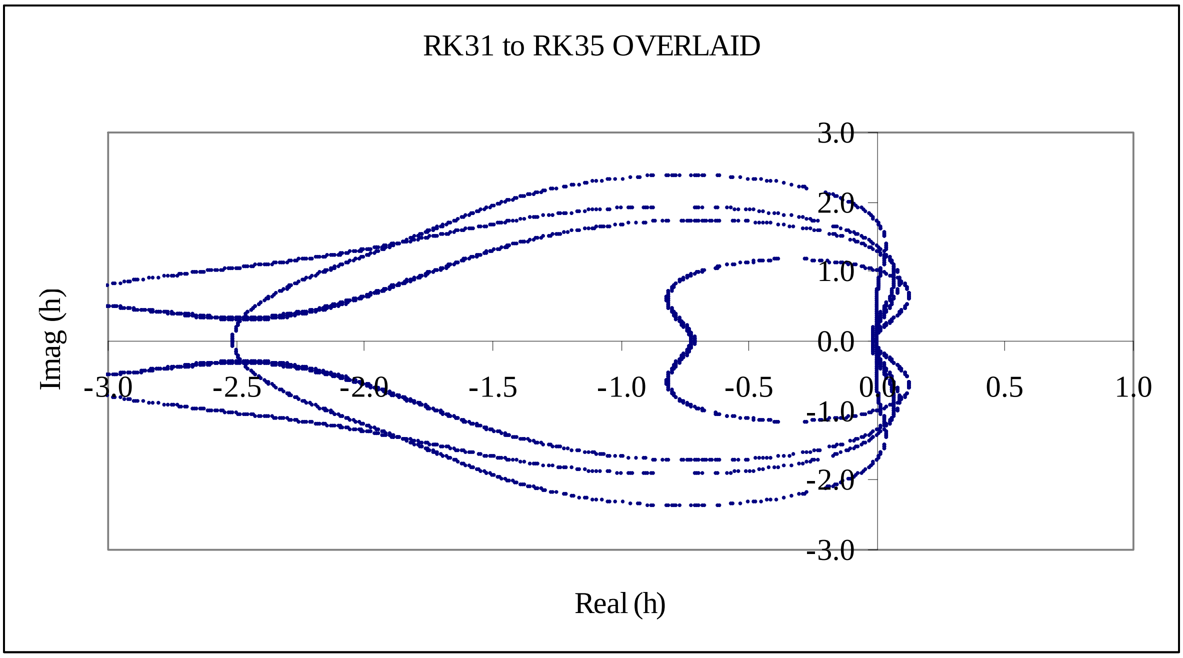

Figure 11: Overlaid stability curves for the third order scheme (RK31 to RK35)

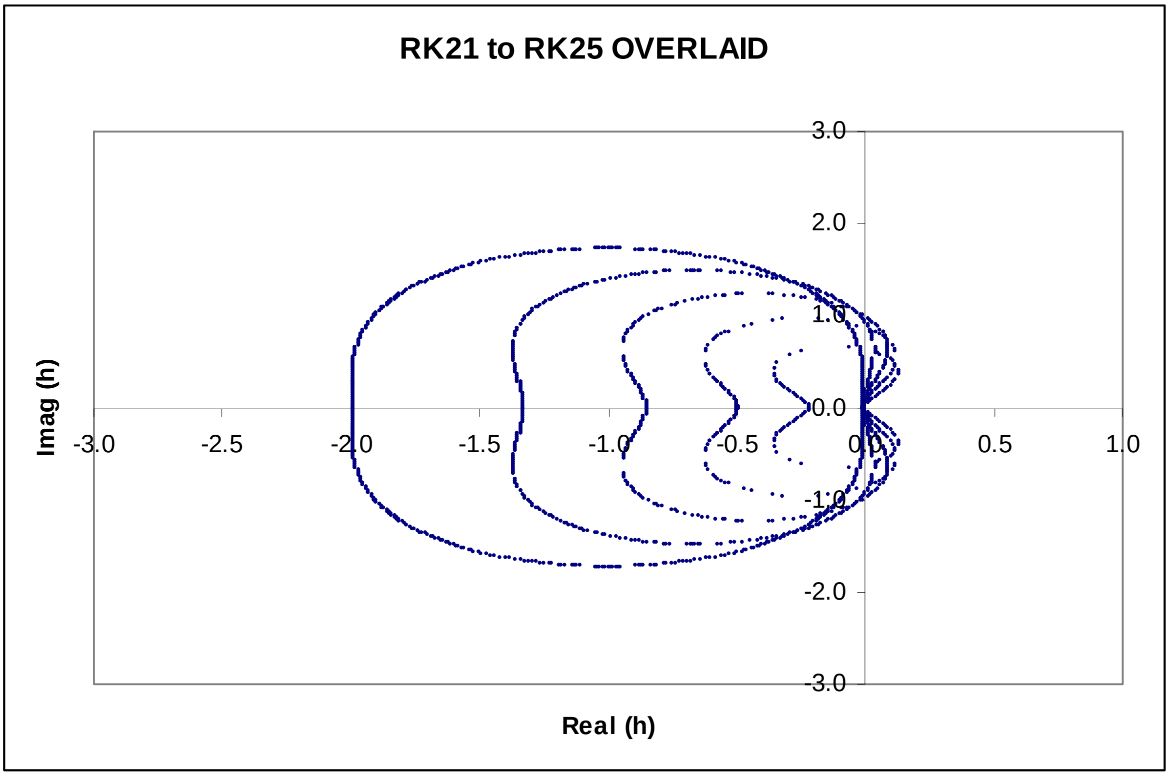

Figure 12: Overlaid stability curves for the second order scheme (RK21 to RK25)

Figures 10 to 12 depicts comparative stable bounded region with respect to studied schemes and five distinct stability polynomials per scheme. Figure 12 shows clearly that the stability domains of the four other versions of the second order scheme studied are subset of the largest stability domain of its popular counterpart. Similar observation of stable region as subset in obscured form is presented in figure 10 and 11 for the fourth and third order scheme respectively.

IV. CONCLUSIONS

The stability polynomial was developed and investigated for the second, third and fourth order Runge-Kutta schemes using the scheme relevant coefficients as input parameters. The combination of the scheme coefficients with increasing power of time step follows a rhyme pattern. The validation test case result agreed perfectly with the test standard result of [1]. Selected studied version of different schemes shows wide variation in the shape of stability curve and stable region bounded. The popular second, third and fourth order schemes have stability curve that bounded larger stable region than their respective counterpart. Thus the study results can be utilised as reliable platform for stability analysis for different version of the second, third and fourth order schemes.

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