

On Redlich-Kister Finite Difference Solution Of Two-Point Boundary Value Problems Using Half-Sweep Kaudd Successive Over Relaxation Iteration

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Abstract — This paper deals with the application of two newly established Redlich-Kister Finite Difference (RKFD) discretization schemes for approximating and solving two-point boundary value problems (TPBVPs). To get the Redlich-Kister Finite Difference Solution of the proposed problem, firstly, two newly second-order half-sweep RKFD discretization schemes are established and used to discretize overall derivative terms of the TPBVPs regarding getting the second-order half-sweep RKFD approximation equation. Then this RKFD approximation equation leads to the construct of the linear system. Due to the increase in the convergence rate iteratively in solving this linear system, the combination of the Kaudd Successive Over Relaxation (KSOR) method with a half-sweep approach is formulated and then known as Half-sweep Kaudd Successive Over Relaxation (HSKSOR) method. With the purpose of evaluating the efficiency of the HSKSOR method, other methods such as Full-sweep Kaudd Successive Over Relaxation (FSKSOR) and Full-sweep Gauss-Seidel (FSGS) are also presented as a control method. The results of the examples of TPBVPs are tested to prove that the HSKSOR iteration is more efficient compared with FSGS and FSKSOR iterations in terms of iterations, execution time, and maximum norm.

Keywords — Boundary value problems, Redlich-Kister Finite Difference scheme, KSOR iteration, Half-sweep concept.

I. INTRODUCTION

Many mathematical models of boundary value problems (BVPs) have been developed in the past few years [1]-[3], especially on TPBVPs. The TPBVPs is one of the mathematical models that have a wide range to its applications either in science, engineering, and physics fields [4]-[6]. Due to its application, this problem has been solved numerically by using numerous numerical techniques [7]-[9]. Following these numerical techniques, the family of spline functions has played an important role in approximating and solving TPBVPs [9]-[10]. For instance, the cubic B-spline function is applied to construct the cubic B-spline approximation equation for solving TPBVPs [11]. Inspired by the application of a family of spline functions, this paper attempts to investigate the capability of two newly established Redlich-Kister Finite

Difference (RKFD) discretization schemes for approximating and solving TBVPs via the Redlich-Kister polynomial function.

In the literature on Redlich-Kister polynomial, commonly, the mathematical models based on Redlich-Kister polynomial can be found for describing the phenomena in physics and chemistry fields [12]-[14]. However, in numerical analysis, only one study has highlighted the development of the piecewise third-order Redlich-Kister polynomial model in which this model gives its high accurate solution as compared to the linear polynomial model [15]. Since there are still big gaps in the literature, therefore many opportunities can be explored to deal with the application of the Redlich-Kister polynomial function as one of the alternative numerical methods to solve any mathematical problem. Apart from using the finite difference schemes in the discretization process, the rapid development of the combination between the standard finite difference schemes with other approaches to form different types of finite-difference discretization schemes, see in [16]-[19]. By taking advantage of the Redlich-Kister polynomial function, this paper initiates in establishing two newly second-order half-sweep RKFD discretization schemes for approximating the TPBVPs and then to construct the corresponding half-sweep RKFD approximation equation.

Based on these discretization schemes being employing in the TPBVPs, the approximation equation leads to generate a large-scale and sparse linear system. According to the properties of the linear system, the iterative methods become the best alternative solver to get efficient solutions [20]-[22]. Due to the simplicity in finding the numerical solution iteratively, up to now, many iterative methods have been developed and applied to seek the solution of this generated linear system [23]-[31]. However, several iterative methods still involve their higher computational complexity. This is because these iterative methods can be classified under the full-sweep iteration family, which requires more computational time to satisfy the convergence criteria. To increase the convergence rate of the full-sweep iteration family by improving the computational complexity, the half-sweep iteration concept needs to be imposed and applied to the generated linear system. The early work on the implementation of this half-sweep iteration concept was originated by [32] to



improve the computational complexity to solve the linear system. Since then, a lot of excellent works have been continued by several researchers to demonstrate its effectiveness and capability to speed up the convergence rate, see in [33]-[37]. With the capability of the half-sweep approach to improving the computational complexity drives to extend the use of this concept, this paper seeks the efficiency of the HSKSOR method for solving the linear system of RKFD approximation equations. This proposed iterative method is the combination of the standard KSOR iterative method together with the half-sweep approach.

Before constructing the two newly established RKFD approximation equation mentioned in the previous paragraph, let consider the general equation of TPBVPs defined as

$$\frac{\partial^2 U}{\partial x^2} + Z(x) \frac{\partial U}{\partial x} + G(x)U(x) = r(x), x \in [0, \phi] \quad (1)$$

with the Dirichlet conditions
 $U(0) = J, U(\phi) = L.$

II. REDLICH-KISTER FINITE DIFFERENCE APPROXIMATION EQUATION

In the first section, this paper considering the Redlich-Kister (RK) polynomial function to construct two newly second-order half-sweep RKFD discretization schemes for approximating the TPBVPs (1). Before performing the discretization process over the proposed problem (1) started, let's consider the RK approximation function of order m as follows

$$U_n(x) = \sum_{k=0}^n a_k \cdot T_k(x) \quad (2)$$

where $a_k, k = 0, 1, 2, \dots, n$ are the unknown parameters to be determined and $T_k(x), k = 0, 1, 2, \dots, m$ represent the Redlich-Kister (RK) function of order k.



Fig. 1 The uniform distribution node points on domain $[0, \phi]$

For the purpose of understanding the process of approximating the TPBVPs (1), let's illustrate the distribution of uniformly grid networks as figured in Fig. 1. According to Fig. 1, the first three RK functions are considered, as seen in Fig. 2.



Fig. 2 The path for T_1, T_2 and T_3

Basically, the implementation of the first three RK functions in Fig. 2 can also be applied over the full- and half-sweep concepts. As figured in Fig. 3, the node points are illustrated for both cases on interval $[0, \phi]$. Based on Fig. 3, and it can be observed that the different values of the subinterval length need to be used for both cases. For

instance, the full-sweep iteration considers the current point to the next point as $1h$, whereas the length of two solid node points for the half-sweep approach is $2h$. It means that when computing the approximate solution, both cases will compute all node points of type \bullet until achieving the convergence criterion. Whereby the direct method is used to compute the remaining node points [32].

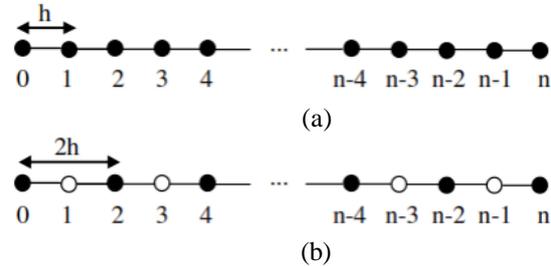


Fig. 3 The uniform distribution points for (a) full-sweep and (b) half-sweep approach

To begin the discretization process via the RK function (2) with a half-sweep iteration concept and considering the RK approximation function of order 2, the following approximation function is considered

$$U(x) = a_0 T_0(x) + a_1 T_1(x) + a_2 T_2(x), \quad (3)$$

where the first three RK functions are defined as

$$\begin{aligned} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_2(x) &= x(1-x). \end{aligned}$$

Since this paper proposed the half-sweep cases as shown in Fig. 3(b), let's define all node points, $x_i = x_0 + ih, i = 0, 2, 4, \dots, n$ where

$$h = \frac{\phi - 0}{n}, n = 2^p, p \geq 1$$

donates the uniform step size based on the finite grid network in Fig. 3. Let's consider a group of three solid node points, x_{i-2}, x_i and x_{i+2} then get

$$U(x_k) = U_k \quad \text{and} \quad T(x_k) = T_k, k = i-2, i, i+2$$

which represented the functions of $U(x)$ and $T(x)$ respectively.

Based on this group of three-node points imposed to equation (3), get the three approximation equations generally as follows

$$U_{i-2} = a_0 T_{0,i-2} + a_1 T_{1,i-2} + a_2 T_{2,i-2}, \quad (4)$$

$$U_i = a_0 T_{0,i} + a_1 T_{1,i} + a_2 T_{2,i}, \quad (5)$$

$$U_{i+2} = a_0 T_{0,i+2} + a_1 T_{1,i+2} + a_2 T_{2,i+2}. \quad (6)$$

After that, by considering all three equations in equation (4) up to (6) and then solved via matrix approach to determine the value of $a_k, k = 0, 1, 2$ in equation (3), it can be shown that the general formulation of the second-order RKFD approximation function can be stated as

$$U(x) = N_0(x)U_{i-2} + N_1(x)U_i + N_2(x)U_{i+2} \quad (7)$$

where $N_k(x), k = 0, 1, 2$ represent the second-order RKFD shape functions, which are defined as

$$\begin{cases} N_0(x) = \frac{1}{8h^2} (x^2 - 2xhi - 2xh + h^2i^2 + 2h^2i), \\ N_1(x) = \frac{1}{4h^2} (2xhi - x^2 - h^2i^2 + 4h^2), \\ N_2(x) = \frac{1}{8h^2} (x^2 - 2xhi + 2xh + h^2i^2 - 2h^2i), \end{cases} \quad (8)$$

Then considering equation (8), the first and second derivative of these RKFD shape functions with respect to can be shown respectively as

$$\begin{cases} N'_0(x) = \frac{1}{8h^2} (2x - 2h - 2hi), \\ N'_1(x) = \frac{1}{4h^2} (2hi - 2x), \\ N'_2(x) = \frac{1}{8h^2} (2x + 2h - 2hi), \end{cases} \quad (9)$$

and

$$\begin{cases} N''_0(x) = \frac{1}{4h^2}, \\ N''_1(x) = -\frac{2}{4h^2}, \\ N''_2(x) = \frac{1}{4h^2}, \end{cases} \quad (10)$$

Then, referring to the RKFD approximation function in equation (7) and applied the first derivative with respect to x_i , the second-order half-sweep RKFD discretization scheme for the first derivative of a function $U(x)$ can be stated as

$$\frac{\partial U}{\partial x} \Big|_i = N'_0(x_i)U_{i-2} + N'_1(x_i)U_i + N'_2(x_i)U_{i+2} \quad (11)$$

Similarly, to get equation (11) by applying the second derivative concept into equation (7) with respect to x_i , the second-order half-sweep RKFD discretization scheme for the second derivative of a function $U(x)$ as follows

$$\frac{\partial^2 U}{\partial x^2} \Big|_i = N''_0(x_i)U_{i-2} + N''_1(x_i)U_i + N''_2(x_i)U_{i+2} \quad (12)$$

As a result, in this paper, both schemes in equations (11) and (12) are referred to as two newly established Redlich-Kister Finite Difference (RKFD) discretization schemes being used to discretize the problem (1). To start doing the discretization process over the proposed problems, let both discretization schemes be imposed over the problem (1) and then the established of half-sweep RKFD approximation equation as follows

$$\alpha_i U_{i-2} + \beta_i U_i + \gamma_i U_{i+2} = r_i \quad (13)$$

where three unknown parameters are given by

$$\alpha_i = N''_0(x_i) + Z_i N''_0(x_i),$$

$$\beta_i = N''_1(x_i) + Z_i N''_1(x_i) + G_i,$$

$$\gamma_i = N''_2(x_i) + Z_i N''_2(x_i).$$

and

$$Z_i = Z(x_i), G_i = G(x_i), r_i = r(x_i), i = 2, 4, 6, \dots, n-2.$$

Now considering all solid node points as depicted in Fig. 3(b) by imposing into equation (13), the construction of the large-scale and sparse linear system in matrix form as follows

$$W \cdot U = r \quad (14)$$

where

$$W = \begin{bmatrix} \beta_2 & \gamma_2 & 0 & 0 & 0 & 0 \\ \alpha_4 & \beta_4 & \gamma_4 & 0 & 0 & 0 \\ 0 & \alpha_6 & \beta_6 & \gamma_6 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \alpha_{n-4} & \beta_{n-4} & \gamma_{n-4} \\ 0 & 0 & 0 & 0 & \alpha_{n-2} & \beta_{n-2} \end{bmatrix},$$

$$U = [U_2 \quad U_4 \quad U_6 \quad \dots \quad U_{n-4} \quad U_{n-2}]^T,$$

$$r = [r_2 - \alpha_2 \cdot J \quad r_4 \quad r_6 \quad \dots \quad r_{n-4} \quad r_{n-2} - \gamma_{n-2} \cdot L]^T.$$

III. DERIVATION OF HSKSOR METHOD

According to the second section, it can be identified that the generated linear system (14) had large-scale and sparse properties. As explained in the first section regarding the properties of the linear system (14), this paper proposed a combination between the standard KSOR method and the half-sweep approach, namely HSKSOR as a linear solver. To construct the HSKSOR method, let's consider the finite grid network and half-sweep concept in Fig. 1 and Fig. 3, respectively. Then, by recalling the coefficient matrix W in equation (14) and rewrite into the three matrices as follows

$$W = T + D + B \quad (15)$$

where D is diagonal, T is lower, and B is an upper matrix of the generated linear system (14). Therefore, the large-scaled and spare linear system (14) can be rewritten as

$$(T + D + B) \cdot U = r \quad (16)$$

Referring to the equation (16), the KSOR method in matrix form as [38]-[39]

$$U^{(q+1)} = [(1-\omega)D - \omega T]^{-1} (D+B)U^{(q)} + [(1-\omega)D - \omega T]^{-1} r \quad (17)$$

where $U^{(q+1)}$ indicate the current value of U at the $(q+1)$ iteration. Again, the KSOR method (17) can also be rewritten in the point iteration approach as follows

$$U_i^{(q+1)} = \frac{1}{(1+\omega)} U_i^{(q)} + \frac{\omega}{(1+\omega)} \left(r_i - \alpha_i U_{i-2}^{(q+1)} - \gamma_i U_{i+2}^{(q)} \right) \quad (18)$$

for $i = 2, 4, 6, \dots, n-2$, whereas the optimum value of ω is different value subject to the size value of n . The range value of ω given [40] by $\omega \in R - [-2, 0]$. Thus, Algorithm 1 describes the summary for the simulation of HSKSOR method in this study.

Algorithm 1: HSKSOR iterative method

- i. Set initial value $U = 0$.
- ii. Calculate the coefficient matrix W and vector, r .
- iii. To $i = 0, 2, 4, \dots, n-2$, calculate the current value

$$U_i^{(q+1)} = \frac{1}{(1+\omega)} U_i^{(q)} + \frac{\omega}{(1+\omega)} \left(r_i - \alpha_i U_{i-2}^{(q+1)} - \gamma_i U_{i+2}^{(q)} \right)$$

- iv. Check the convergence test; if yes, go to step (v). Otherwise, go back to step (iii).
- v. Perform the direct method to compute the approximate solution of the remaining node points
- vi. Display numerical solution.

IV. NUMERICAL EXPERIMENTS AND DISCUSSION

From the formulation in the third section, the HSKSOR iterative method was tested for solving three selected examples of the proposed problem (1). To study the efficiency for the computational performance of the HSKSOR iterative method, other iterative methods, which are FSGS and FSKSOR, are also considered for the sake of comparative analysis. After that, the numerical results of the three iterative methods considered have been analyzed based on three criteria which are the iterations (Iter), execution time (Time) in second and maximum norm (MaxNorm). During the iteration process, the different number of grid sizes are considered, $n = 256, 512, 1024, 2048, 4096$ and the tolerance used is $\varepsilon = 10^{-10}$ for all grid sizes. The following are three examples of TPBVPs and their analytical solution.

Example 1 [41] Consider TPBVPs to be defined as

$$\frac{\partial^2 U}{\partial x^2} - \frac{\partial U}{\partial x} = -e^{(x-1)^{-1}}, \tag{19}$$

The analytical solution of equation (19) is $U(x) = x \left(1 - e^{(x-1)} \right)$.

Example 2 [42] Consider TPBVPs be stated as

$$\frac{\partial^2 U}{\partial x^2} + U(x) = -1, \tag{20}$$

The analytical solution of equation (20) is $U(x) = \cos(x) + \frac{1 - \cos(1)}{\sin(1)} \sin(x) - 1$.

Example 3 [8] Consider TPBVPs be stated as

$$\frac{\partial^2 U}{\partial x^2} - 4U = \cosh(1), \tag{21}$$

The analytical solution of equation (21) is $U(x) = \cos(2x - 1) - \cosh(1)$.

The results from the simulation of FSGS, FSKSOR, and HSKSOR iterative methods based on Algorithm 1 were tabulated in Tables 1 to Table 3 then Table 4 shows that the reduction percentage of FSKSOR and HSKSOR for all numerical examples are considered.

TABLE 1 THE RESULTS FOR EXAMPLE 1 BASED ON COMPARISON CRITERIA CONSIDERED

n	Method	Iter	Time(second)	Error
256	FSGS	82043	7.92	4.0343e-07
	FSKSOR	769	0.75	2.4866e-07
	HKSOR	389	0.16	9.8784e-07
512	FSGS	292276	16.23	2.5291e-06
	FSKSOR	1526	1.67	6.7370e-08
	HKSOR	769	0.37	2.4521e-07
1024	FSGS	1025489	76.67	1.0346e-05
	FSKSOR	2853	3.19	2.5732e-08
	HKSOR	1526	0.86	6.7345e-08
2048	FSGS	3527433	409.03	4.1443e-05
	FSKSOR	5792	6.63	1.7614e-08
	HKSOR	2849	1.64	2.6076e-08
4096	FSGS	11811519	2359.09	1.6579e-04
	FSKSOR	10221	10.41	9.8302e-08
	HKSOR	5791	3.36	1.7686e-08

TABLE 2 THE RESULTS FOR EXAMPLE 2 BASED ON COMPARISON CRITERIA CONSIDERED

n	Method	Iter	Time(second)	Error
256	FSGS	89973	19.88	5.4091e-07
	FSKSOR	782	0.37	1.9062e-07
	HKSOR	398	0.18	7.9533e-07
512	FSGS	318924	60.80	2.9059e-06
	FSKSOR	1537	0.89	5.2948e-08
	HKSOR	782	0.47	1.9062e-07
1024	FSGS	1111808	256.86	1.1810e-05
	FSKSOR	3057	1.82	1.5546e-08
	HKSOR	1537	0.87	4.3126e-08
2048	FSGS	3791677	1260.25	4.7285e-05
	FSKSOR	5734	3.43	2.5772e-08
	HKSOR	3057	1.92	1.5546e-08
4096	FSGS	13659733	7301.95	1.7907e-04
	FSKSOR	10655	5.78	1.0642e-07
	HKSOR	5734	3.36	2.5772e-08

TABLE 3 THE RESULTS FOR EXAMPLE 3 BASED ON COMPARISON CRITERIA CONSIDERED

n	Method	Iter	Time(second)	Error
256	FSGS	66139	13.96	2.4092e-06
	FSKSOR	720	0.82	1.9355e-06
	HKSOR	382	0.19	7.7476e-06
512	FSGS	238353	44.83	2.3742e-06
	FSKSOR	1353	1.38	4.7876e-07
	HKSOR	720	0.37	1.9355e-06
1024	FSGS	848604	184.48	7.6812e-06
	FSKSOR	2609	2.78	1.0851e-07
	HKSOR	1353	0.85	4.7876e-07
2048	FSGS	2975185	927.17	3.0271e-05
	FSKSOR	4908	5.11	1.9449e-08
	HKSOR	2799	1.61	1.2885e-07
4096	FSGS	10223821	2150.65	1.2097e-04
	FSKSOR	9162	9.23	6.7222e-08
	HKSOR	4908	3.16	1.9449e-08

TABLE 4 REDUCTION PERCENTAGE FOR THE KSOR AND HSKSOR IN TERM OF THE ITERATION AND TIME

		KSOR (%)	HSKSOR(%)
Exam ple 1	I	99.06-99.84	99.53-99.95
	Time	89.71-99.56	95.83-99.86
Exam ple 2	I	99.13-99.92	99.56-99.96
	Time	98.13-99.92	99.09-99.95
Exam ple 3	I	98.91-99.91	99.42-99.95
	Time	94.13-99.57	98.64-99.85

From all numerical results by imposing FSGS, FSKSOR, and HSKSOR iterative methods as shown in Table 1 up to 4, it clearly shows that the combination of KSOR iterative method with half-sweep approach gives less iteration and Time compared to the FSGS and FSKSOR methods. For instance, in terms of iteration for solving Example 1, it can be pointed out that the HSKSOR method has declined approximately 99.53-99.95% when compared to the FSGS method, whereas the FSKSOR iterative method has approximately 99.06-99.84%. Also, in terms of Time, the HSKSOR method is faster, about 95.83-99.86%, than the FSGS iteration, whereas the FSKSOR iteration has about 89.71-99.56%. In the meantime, it can be observed that the pattern of reduction percentage for Example 2 and Example 3 is the same as Example 1, which is the HSKSOR iterative method shows the highest reduction percentage compared to the other two iterative methods. In conclusion, the HSKSOR method requires the least iteration and Time as compared to FSGS and FSKSOR methods. From the accuracy of iterative methods considered, the numerical solution of the FSKSOR and HSKSOR methods are in good agreement and close to their analytical solution compared to the FSGS iterative method

V. CONCLUSIONS

This paper has successfully derived the formulation of FSGS, FSKSOR, and HSKSOR iterative methods by applying the two newly established RKFD discretization schemes. According to the numerical results obtained by solving three examples of TPBVP, clearly numerical results have pointed out that the FSKSOR method gives less iteration and Time as compared to the FSGS method. However, the application of the half-sweep approach into the KSOR iterative method, HSKSOR, could give the least iteration and Time when compared with both considered iterative methods. Meanwhile, the accuracy of FSKSOR and HSKSOR iterative methods are comparative same, but also the accuracy of their solutions is more accurate than FSGS iteration at all grid sizes. Therefore, the conclusion is the HSKSOR method is a superior method compared to FSGS and FSKSOR methods. For further works, this paper should be continued to investigate the application of these

two newly established RKFD discretization schemes for approximating and solving the multi-dimensional boundary value problem by using the two-step iteration family [43]- [44] and the families of half-sweep [39],[45] and quarter-sweep [46]-[48] approaches.

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