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A SOR METHOD UTILIZING REDLICH-KISTER FINITE DIFFERENCE FOR TWO POINT BOUNDARY VALUE PROBLEMS

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ABSTRACT. *This study presents a numerical method using a second-order Redlich-Kister Finite Difference (RKFD) discretization scheme to approximate the two-point boundary value problems (TPBVPs). The approach creates a linear system for the given problem by using the first two derivatives to create the RKFD approximation equation. Two iterative approaches are used to solve the linear system: Gauss-Seidel (GS) and Successive Over-Relaxation (SOR). Two model examples that assess each approach according to its number of iterations, execution time, and maximum norm over five different mesh sizes indicate the effectiveness of these proposed iterative methods. The results show that the SOR method outperforms the GS methods in providing an extremely accurate approximation of the known exact solution.*

INTRODUCTION

In recent years, there has been increasing interest in creating, applying, and studying numerical methods for boundary value problems due to the difficulties in deriving analytical solutions (Aarao *et al*., 2010). One such equation, the two-point boundary value problem, has widespread applications in science, engineering, and physics research areas (Gupta, 2012; Wang & Guo, 2008). Many researchers have devoted their efforts to designing accurate numerical solutions for TPBVPs and recognize the difficulties associated with obtaining them. Previous studies have explored various numerical techniques to address the TPBVPs. Mohsen and El-Gamel (2008) used the Galerkin and collocation methods to numerically simulate this problem, while Liu *et al*. (2011) proposed a polynomial spline implementation as a numerical solution. Furthermore, researchers have investigated a B-spline method (Caglar & Caglar, 2009) to tackle the diffusion problem. Additionally, the literature provides a range of other numerical solutions for TPBVPs (Al-Towaiq, 2023; Pandey, 2023; Rashidinia & Sharifi, 2015; Wang, 2023; Zhanlav *et al*., 2024), which can be applied to the study of TPBVPs.

Based on the method mentioned in the previous paragraph, we propose a new approach called the RKFD method to solve the boundary value problem. This method is based on the Redlich-Kister (RK) function, which is widely used in physics and chemistry to obtain solutions but has been less commonly utilised in other fields (Babu *et al*., 2019; Gayathri *et al*., 2019; Komninos & Rogdakis, 2020). Over time, its application has been extended to solve numerical analysis problems. The background of this method in numerical analysis started with the study (Hasan *et al*., 2010), in which the piecewise RK polynomial model has been used, focusing on the construction of first- and third-order models and on analysing the relationship between Gauss-Seidel iteration and mesh sizes. The findings indicated that the third Redlich-Kister model offers good accuracy compared to the first model.

Following this research, subsequent research has gone deeper into the application of RK functions to numerical analysis fields. For example, in Suardi and Sulaiman (2021b), the authors suggested the use of RK polynomials to solve a one-dimensional boundary value problem. Furthermore, Suardi & Sulaiman (2021a, 2022) proposed RKFD, which combines the RK polynomial and finite difference methods to solve a problem of two-point boundary value problems. The use of the RKFD approximation equation generates the system of the RKFD equation, which will be solved by iterative methods, which is the SOR method, as a linear solver. In literature, Young (1970) explored the various SOR methods for solving linear equation systems of $Au = b$ and discovered that the SOR methods with optimal relaxation parameters produce small radio waves. In addition, Sampoorna and Bueno (2010) tested the partial atomic redistribution problems by using the Gauss-Seidel method and the SOR, and they then found that the SOR method could solve the problem in a short time. This is supported by Radzuan *et al*. (2018), who mentioned that the SOR method can accelerate the convergence of linear equation solutions using optimal relaxation parameters. Inspired by all those studies, the paper aims to develop numerical solutions for problems involving TPBVPs in Equation 1.

$$\frac{d^2U}{dx^2} + Z(x)\frac{dU}{dx} + G(x)U(x) = r(x) \tag{1}$$

With the Dirichlet conditions

$$U(0) = \varphi_0, U(\phi) = \varphi_1.$$

RKFD APPROXIMATION EQUATION

Before the numerical process begins for Equation 1, the two newly established RKFD approximation equations must be constructed, as described in the preceding section. To construct these approximation equations, a discretisation process based on the Redlich–Kister (RK) function is required. Defining the general formula of the RK function is in Equation 2.

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

where $a_k, k = 0,1,2,\ldots,n$ are the unknown parameters.

Before calculating the unknown parameters in equation 2, the distribution of the mesh sizes utilised is depicted in Figure 1. The size of the mesh shown in Figure 1 provides an understanding of the formulation of the first three Redlich-Kister (RK) functions, as depicted in Figure 2.

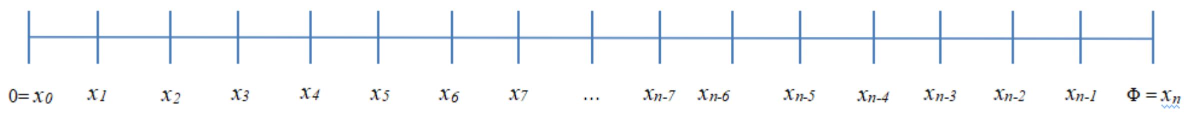

Figure 1. Distribution of mesh sizes considered.

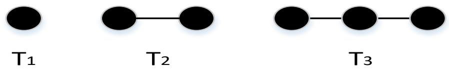

Figure 2. The path for T_0, $T_{1,}$ and T_2.

Applying the concept of Figure 2 to Equation 2 can mean that the second-order RK approximation function is expressed in Equation 3.

$$U(x) = a_0T_0(x) + a_1T_1(x) + a_2T_2(x) \tag{3}$$

Where the first three RK functions are defined as

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = x(1-x).$$

Then, the grid network shown in Figure 1 is set up as a reference domain for equation 3 by applying the node points, $x_c = x_0 + ch, c = 0,1,2,\dots,n$ and defining the uniform step size as $h = \frac{\varphi-0}{n}, n = 2^p, p \geq 1$. This process is used to solve the following linear system and obtain unknown parameters in equation 3.

$$\begin{bmatrix} U_{c-1} \\ U_c \\ U_{c+1} \end{bmatrix} = \begin{bmatrix} T_0(x_{c-1}) & T_1(x_{c-1}) & T_2(x_{c-1}) \\ T_0(x_c) & T_1(x_c) & T_2(x_c) \\ T_0(x_{c+1}) & T_1(x_{c+1}) & T_2(x_{c+1}) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}, \tag{4}$$

where $\mathrm{U(x_c)} = \mathrm{U_c}$. After that, Equation 4 is solved using the matrix approach to derive the formulas for the three unknown parameters in Equation 3. Equation 3 was used to replace all three parameters and rewrite them as Equation 5.

$$U(x) = N_0(x)U_{c-1} + N_1(x)U_c + N_2(x)U_{c+1} \tag{5}$$

where the RKFD shape functions, $N_k(x), k = 0,1,2$ can be defined as Equation 6.

$$\left.\begin{aligned} N_0(x) &= (x^2 - 2xhc - xh + h^2c^2 + h^2c)/(2h^2) \\ N_1(x) &= (2xhc - x^2 - h^2c^2 + h^2)/(h^2) \\ N_2(x) &= (x^2 - 2xhc + xh + h^2c^2 - h^2c)/(2h^2) \end{aligned}\right\} \tag{6}$$

By evaluating the first and second derivatives concept on Equation (6), the RKFD approximation function is expressed as Equation 7.

$$\left.\begin{aligned} \frac{dU}{dx}\bigg|_c &= N_0'(x_c)U_{c-1} + N_1'(x_c)U_c + N_2'(x_c)U_{c+1} \\ \frac{d^2U}{dx^2}\bigg|_c &= N_0''(x_c)U_{c-1} + N_1''(x_c)U_c + N_2''(x_c)U_{c+1} \end{aligned}\right\} \tag{7}$$

where $U(x_c) = U_c, c = 0,1,2,\dots,n$ accorded as the approximation solution of the function U(x). The expression generated by equation 7 highlights the two newly established RKFD discretisation methods, which correspond to the primary objective of this work. These approaches have been designed for constructing the RKFD approximation equation to solve the suggested problem (1). By substituting equation 7 into the given problem and applying the second-order central difference techniques for discretising in time, a second-order RKFD approximation, Equation 8, could be constructed as follows for the TPBVP

$$\alpha_cU_{c-1} + \beta_cU_c + \gamma_{c+1}U_{c+1} = R_c, \tag{8}$$

where

$$\alpha_c = N_0''(x_c) + ZN_0'(x_c), \beta_c = N_1''(x_c) + ZN_1'(x_c) + G_c, \gamma_c = N_2''(x_c) + ZN_2'(x_c)$$

Next, the RKFD linear systems can then be built in matrix form using the RKFD approximation equation 8 as follows:

$$W \cdot \underline{U} = \underline{R} \tag{9}$$

DERIVATION OF SOR ITERATIVE METHOD

From the previous section, the generated large-scale and sparse linear systems (9) emerge as a result of the completed RKFD discretisation scheme process. Based on many research studies (Hackbusch, 1994; Saad, 2003; Young, 2014), it is recommended to use iterative methods to solve this linear system since it involves a large scale within the coefficient matrix. To solve equation 9 in this study, the SOR iterative approach has been regarded as a linear solution. Studies on the application and effectiveness of the SOR method, which is an enhancement of the GS method, have been conducted by Kalambi (2008) and Youssef (2012). When applying the SOR approach, which is impacted by the weighted parameter's value determination, the range should be $1 \leq \omega \leq 2$. However, when the weighted parameter is taken as equal to one, $\omega = 1$the SOR method will change into the GS method (Equation 10) (Kalambi, 2008).

$$(F + J + L) \cdot \underline{U} = \underline{R}, \tag{10}$$

where J, F and L are diagonal matrix, triangular lower and upper matrices. Through manipulation of equation 10, the representation of the SOR method in the form of a point iteration form is presented in Equation11.

$$\underline{U}^{(q+1)} = (1 - \omega)\underline{U}^{(q)} + \omega(J + F)^{-1}\left(\underline{R} - L\underline{U}^{(q)}\right) \tag{11}$$

where $\underline{U}^{(q+1)}$ referring to the value of $U(x)$ at the $(q + 1)^{th}$ iteration.

NUMERICAL PROBLEM AND DISCUSSION

In the previous discussion, the RKFD approximation equation was derived, and the numerical experiment was conducted to solve problem (1) using the SOR method. To determine the applicability of the suggested method, two examples were tested with different mesh sizes, $n = 256,512,1024,2048,4096$. Additionally, numerical comparisons were done in terms of the number of iterations (Iter), execution time (Time), and maximum norm. Following that, a tolerance error, $\varepsilon = 10^{-10}$ is always used for all examples that are taken into consideration.

Example 1
The TPBVPs (1) as (Caglar *et al.*, 2006)

$$\frac{d^2U}{dx^2} - \frac{dU}{dx} = -e^{(x-1)^{-1}} \tag{12}$$

and the analytical solution of problem (12) is $U(x) = x\left(1 - e^{(x-1)}\right)$.

Example 2
The TPBVPs (1) with as (Ramadan *et al.*, 2007)

$$\frac{d^2U}{dx^2} - U(x) = -1 \tag{13}$$

and the analytical solution of problem (13) is $U(x) = \cos(x) + \frac{1-\cos(1)}{\sin(1)}\sin(x) - 1$.

As predicted in Table 1, the numerical result indicates that the SOR method with the RKFD approximation equation outperforms the GS method, the benchmark method in this study, in terms of iteration and time. The SOR method can generate fewer iterations and converge more quickly across all examples tested. For instance, in Table 1, 769 iterations are required by the SOR method and 0.73 seconds to converge Example 1 at a 256 mesh size, while the GS method required 82043 iterations and 22.54 seconds. The advantage of the SOR method becomes more pronounced as the mesh size increases, as seen in the results for n = 4096, where the SOR method required 10244 iterations and 10.51 seconds, compared to the GS method, which required 11811519 iterations and 2359.09 seconds. The numerical results for solving problems exhibit a similar pattern, with the SOR method demonstrating improved performance over the GS method, as reported in Example 2. These findings are consistent with the literature (Suardi & Sulaiman, 2022), which indicates that the SOR method can enhance the applicability of the GS method for solving TPBVPs. In terms of accuracy, both the SOR and GS methods showed excellent agreement with their respective exact solutions.

Table 1. Numerical results for examples 1 and 2.

n	Method	Example 1			Example 2		
		Iter	Time	MaxNorm	Iter	Time	MaxNorm
256	GS	82043	22.54	4.0343e-07	89973	19.88	5.4091e-07
	SOR	769	0.73	2.4519e-07	769	0.39	2.0467e-07
512	GS	292276	35.51	2.5291e-06	318924	60.80	2.9059e-06
	SOR	1526	1.57	6.7390e-08	1537	0.88	4.3126e-08
1024	GS	1025489	117.83	1.0346e-05	1111808	256.86	1.1810e-05
	SOR	2946	3.46	1.9947e-08	3057	1.81	1.5554e-08
2048	GS	3527433	409.02	4.1443e-05	3791677	1260.25	4.7285e-05
	SOR	5792	6.64	1.7364e-08	5733	3.44	2.5779e-08
4096	GS	11811519	2359.09	1.6579e-04	12544476	2681.69	1.8915e-04
	SOR	10244	10.51	9.3638e-08	10660	5.71	1.0453e-07

CONCLUSION

The GS and SOR methods are looked at in this paper as two iterative ways to get the numerical solution of two new RKFD approximation equations for solving TPBVPs. Firstly, the problem was discretised to form the RKFD approximation equation. The resulting linear system was then solved using the considered iterative methods. To validate the applicability of the iterative methods, two examples were tested, and the numerical results revealed that the SOR method produces the lowest number of iterations and is faster than the GS method. This conclusion was drawn from the analysis of the comparison of both methods presented in Table 1, which demonstrates the superior performance of the SOR method compared to the GS method.

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