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The Technique of Discontinuity Tracking Equations for Functional Differential Equations in 1-Point Implicit Method

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ABSTRACT

In this paper, we proposed to deal with the derivative discontinuities in the numerical solution of functional differential equation by using the technique of discontinuity tracking equations. This technique will be adapted in a linear multistep method with the support of Runge-Kutta Felhberg step size strategy. Naturally, the existence of discontinuities will produce a large number of failure steps that can lead to inaccurate results. In order to get a smooth solution, the technique of detect, locate and treat of the discontinuities has been done in the developed algorithm. The numerical results has shown that this technique not only can improve the solution in terms of smoothness but it also enhance the efficiency and accuracy of the proposed method.

Keywords: Derivative of Discontinuity; Retarded Functional Differential Equations; Runge-Kutta Felhberg; linear multistep method

1. INTRODUCTION

The assumption of the solution to be sufficiently smooth is very important for solving differential equations in any numerical methods. Usually, the non-smooth solution occurs when the local truncation errors which form the basis of the step size selection algorithm is no longer valid. One of the phenomena that may arise in this problem is the presence of derivative discontinuities which may exist in functional differential equations (FDE) in various time-scales. Let consider the FDE with the solution of the left-hand and the right-hand derivative which do not agree at $x_0 = a$ i.e. $\phi'(x_{a^-}) \neq y'(x_{a^+})$, for

$$y'(x) = f(x, y(x), y(x-\tau(x))), \qquad x \in [a,b], \qquad (1)$$

with the following initial function,

$$y(x) = \phi(x), \qquad x \in [-\tau, a],$$

where f and ϕ are the given functions, $(x-\tau(x))$ is the retarded term with τ is a positive constant and $y(x)$ is the unknown function that need to be found in the interval $[a,b]$.

The study of discontinuities was initially arise when there exist a jump in the solution that might give the large effect on the accuracy when solving a particular ordinary differential equations

(ODE). By realizing that, Carver (1978) has developed a new method of detecting and handling discontinuities in arbitrary functions of ODE where the method has been implemented by Gear (1970) for solving the sets of stiff equation. In 1981, Ellison was then classified discontinuities in two major types known as time and state events and has developed a new approach in detecting the location of state events using Hermite interpolation.

In functional differential equations, Neves (1975) has suggested two ways in treating discontinuities which are by ignoring them and then depending on the local error control mechanism; or stopping the integration at the discontinuity point and then requiring the user to restart the integration. However, the strategy to ignore the discontinuities is not really recommended because it can waste the computing time and does not give a reliable results, see Hairer et al. (1987).

Besides, Enright & Hayashi (1997) has adapted the technique for initial value ordinary differential equations which is called defect error control in handling derivative discontinuities for delay differential equations (DDE). Then, Paul (1999) has implemented the technique of discontinuity tracking equations in the Runge-Kutta method that has been initialized by Baker & Wille (1988). This technique can be implemented by giving the position of the discontinuity at the initial point, then the position of the propagated discontinuity can be found by solving the nonlinear equations of the form $s_i - \tau(s_i, y(s_i)) = s_j$. Here, s_j corresponds to a previous discontinuity and s_i is the same point of discontinuity where the approximation to s_i is refined as the solution progress.

In linear multistep method, the strategy in treating the small delay case in the retarded type of functional differential equations has been proposed by Aziz & Majid (2014, 2015). In their study, they only focus on how to handle the small and vanishing delay that has been disappeared in the solution. Besides the one-step and multistep method, Li and Zhang (2014) also has investigated the error estimation of derivative discontinuity in Galerkin method while Lenz et al. (2014) developed the experimental solver namely COLSOL-DDE in treating this case.

Therefore, in this paper we are intent to adapt the technique so-called discontinuity tracking equations that has been proposed by Baker and Wille (1988) for handling the derivative discontinuities of functional differential equations in linear multistep method that has been proposed in Majid & Suleiman (2006). This technique has been support with the implementation of Runge-Kutta Felhberg step size strategy in order to enhance the efficiency of the method and getting the smooth solution along the integration.

2. 1-POINT IMPLICIT METHOD

In this paper, we will consider the 1-point implicit method that has been proposed by Majid and Suleiman (2006). This method can be defined in the standard form as

$$\sum_{j=0}^{k} \alpha_j y_{n+j-3} = h \sum_{j=0}^{k} \beta_j f_{n+j-3}, \qquad (2)$$

where α_j and β_j are constants subject to the conditions $\alpha_k = 1,\ \alpha_{k-1} = -1$ and $\alpha_j = 0$ for $j = 0,1,2.$ The method of (2) is said to be explicit if $\beta_k = 0$ and implicit if $\beta_k \neq 0$ where having $j = 0$ until $k = 4$ is the number of steps taken for predictor and corrector formula.

The derivation of the method starts by considering the initial value problem (IVP) of ordinary differential equations (ODEs) as follows,

$$y'(x) = f(x, y), \qquad y(a) = y_0, \qquad a \le x \le b. \tag{3}$$

In order to determine the solution of $y_{n+1}(x)$, the IVP in (3) is then will be integrated over the interval $[x_n, x_{n+1}]$ as follows,

$$\int_{x_n}^{x_{n+1}} y'(x)dx = \int_{x_n}^{x_{n+1}} f(x, y)dx, \qquad \text{or} \qquad y_{n+1}(x) - y_n(x) = \int_{x_n}^{x_{n+1}} f(x, y)dx, \tag{4}$$

where $f(x, y)$ in the integral can be replaced by the Lagrange polynomial $P_q(x)$ of degree q.

Predictor:

$$\begin{aligned} y(x_{n+1}) - y(x_n) &= \int_0^1 P_3(x)dx \\ &= h\int_0^1 \frac{(s+m+q+r)(s+q+r)(s+r)}{(m+q+r)(q+r)(r)} ds(f_n) \\ &+ h\int_0^1 \frac{(s+m+q+r)(s+q+r)(s)}{(m+q)(q)(-r)} ds(f_{n-1}) \\ &+ h\int_0^1 \frac{(s+m+q+r)(s+r)(s)}{(m)(-q)(-1)(q+r)} ds(f_{n-2}) \\ &+ h\int_0^1 \frac{(s+q+r)(s+r)(s)}{(-m)(-1)(m+q)(-1)(m+q+r)} ds(f_{n-3}). \end{aligned} \tag{5}$$

Corrector:

$$\begin{aligned} y(x_{n+1}) - y(x_n) &= \int_{-1}^0 P_4(x)dx \\ &= h\int_{-1}^0 \frac{(s+m+q+r+1)(s+q+r+1)(s+r+1)(s+1)}{(m+q+r+1)(q+r+1)(r+1)} ds(f_{n+1}) \\ &+ h\int_{-1}^0 \frac{(s+m+q+r+1)(s+q+r+1)(s)}{(m+q+r)(q+r)(-r)} ds(f_n) \\ &+ h\int_{-1}^0 \frac{(s+m+q+r+1)(s+q+r+1)(s+1)(s)}{(m+q)(q)(-r)(-1)(r+1)} ds(f_{n-1}) \\ &+ h\int_{-1}^0 \frac{(s+m+q+r+1)(s+r+1)(s+1)(s)}{(m)(-q)(-1)(q+r)(-1)(q+r+1)} ds(f_{n-2}) \\ &+ h\int_{-1}^0 \frac{(s+q+r+1)(s+r+1)(s+1)(s)}{(-m)(-1)(m+q)(-1)(m+q+r)(-1)(m+q+r+1)} ds(f_{n-3}). \end{aligned} \tag{6}$$

Since, the Runge-Kutta Felhberg step size strategy will be adapted in this solution, therefore the step size ratios *r*, *q* and *m* in (5) and (6) will be substituted with any values by depending on the formula in Section 4. This strategy implies different coefficients in the predictor and corrector formula that will reduce the computational work.

3. DISCONTINUITY TRACKING EQUATION

In the numerical solution of FDE, it is very significant for one to understand the way of how the discontinuities being propagated by the delays $\tau(x)$. The difficulty to treat it is highly rely on the function of retarded term either it is a constant, time-dependent or state-dependent function delays. For the sake of simplicity, let consider the constant retarded term of FDE with discontinuity at first derivative i.e. $\phi'(x_{0-}) = 0 \neq 1 = y'(x_{0+})$,

$$\begin{aligned} y'(x) &= y(x-1), && x \geq 0, \\ y(x) &= 1, && x \leq 0, \end{aligned} \tag{6}$$

with the discontinuity tracking equations give in the form of

$$s_i - \tau(s_i, y(s_i)) = s_j. \tag{7}$$

Our aim is to obtain the approximation of s_i which are some points of derivative discontinuities that will propagated from the initial point. By solving equation (17), we will have $x_r - 1 = x_{r-1}$ for $x_r > x_{r-1}$ with *r*-th is the derivative and thus, $x_r = x_{r-1} + 1$ for $r > 0$. The solution in each subinterval can be obtained by integrating $y'(x) = 1$ and substitute $x = 0$ in $y(x)$, we have $y(x) = x + 1$ for the interval $[0,1]$. Repeating the same procedure, we will obtain the solution as follows,

Interval $[0,1]$**:** $y'(x) = 1,$ so that $y(x) = x + 1.$

Interval $[1,2]$**:** $y'(x) = (x-1) + 1,$ so that $y(x) = \frac{1}{2}x^2 + \frac{3}{2}.$

Interval $[2,3]$**:** $y'(x) = \frac{1}{2}(x-1)^2 + \frac{3}{2},$ so that $y(x) = \frac{1}{6}x^3 - \frac{1}{2}x^2 + 2x + \frac{1}{6}.$

Thus, we can see that there is a jump of discontinuities in second derivatives $y''(1^-) = 0 \neq 1 = y''(1^+)$ that has being propagated from $x = 0$ and the jump in third derivatives $y'''(2^-) = 0 \neq 1 = y'''(2^+)$ and so on.

Since the discontinuity points are detected earlier, so it is easier to include the discontinuity points in the mesh point. This is purposely to get a continuously smooth solutions that lead to the better accuracy and fewer rejected steps. The step size is then be restricted as $x_{n+1} + h \leq \zeta_i$ where ζ_i is discontinuity point for $i = 1,2,3$. The integration is then are set to be restarted with the new function in particular subintervals using sufficiently small step size as $h = 1.0^{-15}$.

4. Runge-Kutta Felhberg Step Size Strategy

In dealing with the derivative of discontinuities, one should consider the best strategy of the chosen step size along the interval. So that, the solution will have the optimum step size that allow the discontinuity points to be included in the mesh point. For this reason, the strategy of Runge-Kutta Felhberg has been adapted to vary the h since the more options of step size can be implemented in getting the best accuracy of the method.

Lets denote h_i as the initial step size, h_{old} as the most recent step size, h_{new} as the next step size that need to be determined, $h_{\min}$ as the minimum step allowed by the routine, TOL as the tolerance per unit step, EQN as the number of equations, $DMAX$ as the initial function evaluation, $MAXE$ as the maximum of mixed error test for $A = B = 1$, $SSTEP$ as the number of successful step and $p = 1$ is for 1-point implicit method. The algorithm of this strategy is described as follows.

Step 1: Set TOL and $h_{\min} = 1.E-15$.

Step 2: Calculate the initial step size, $h_i = \dfrac{\left(\dfrac{TOL}{DMAX}\right)^{\frac{1}{EQN+1}}}{4.0^{EQN}}$.

$$h_i = h_i * 1.E-5.$$

Step 3: Compute the estimate $E_{p,k}$ per unit step, using

$$E_{p,k} = \left| y_{n+p}^{(k)} - y_{n+p}^{(k-1)} \right|.$$

Step 4: Compute the maximum error,

$$MAXE = \max_{1 \le i \le SSTEP} \left\{ \max_{1 \le i \le N} \left| \frac{y_{n+p} - y(x_{n+p})}{A + By(x_{n+p})} \right| \right\}.$$

Step 5: If $(E_{p,k} \le TOL)$, ***Successful Step***

Set $HACC = 0.8\left(\dfrac{TOL}{E_{p,k}}\right)^{\frac{1}{4}}$.

If $HACC < 0.1$, then $h_{new} = 0.1 * h_{old}$.

Else if $HACC > 4.0$, then $h_{new} = 4.0 * h_{old}$.

Else $h_{new} = HACC * h_{old}$.

Step 6: Else, ***Failure Step***

Set $h_{new} = 0.5 * h_{old}$.

Step 7: Compute the step size ratio,

$$r = \frac{h_{old}}{h_{new}}, \quad q = r_{old}\left(\frac{h_{old}}{h_{new}}\right), \quad m = q_{old}\left(\frac{h_{old}}{h_{new}}\right).$$

5. NUMERICAL RESULT AND DISCUSSION

In this section, we have tested two discontinuity problems of FDE for the type of constant and time-dependent retarded term. The algorithm has been performed using Microsoft Visual C++ 6.0 program and the numerical results will be compared by according to with and without discontinuity tracking equations strategy.

Problem 1:

$$\begin{aligned} y'(x) &= y(x-1), && x \geq 0, \\ y(x) &= 1, && x \leq 0, \end{aligned}$$

with the exact solution

$$y(x) = \begin{cases} x+1, & [0,1], \\ \frac{1}{2}x^2 + \frac{3}{2}, & [1,2], \\ \frac{1}{6}x^3 - \frac{1}{2}x^2 + 2x + \frac{1}{6}, & [2,3]. \end{cases}$$

Problem 2:

$$\begin{aligned} y'(x) &= y(x-\frac{1}{x}), && x \geq 0, \\ y(x) &= 1, && x \leq 0, \\ y(0) &= 0, \end{aligned}$$

with the exact solution

$$y(x) = \begin{cases} x, & [0,1], \\ \frac{1}{2}x^2 - \ln(x) + \frac{1}{2}, & [1, \frac{1}{2}(1+\sqrt{5})], \\ \frac{1}{6}x^3 + \frac{1}{2}x - \frac{1}{2x} - x\ln(x-\frac{1}{x}) + \frac{5}{12} + \frac{\sqrt{5}}{12} - \ln\left(\frac{1}{2}\left(3-\sqrt{5}\right)\right), & [\frac{1}{2}(1+\sqrt{5}), \frac{1}{4}(1+\sqrt{5}+\sqrt{22+2\sqrt{5}})]. \end{cases}$$

The end point for these problems is only restricted to $x=3$ and $x=\frac{1}{4}(1+\sqrt{5}+\sqrt{22+2\sqrt{5}})$ respectively where the solution is available up until this point only. Solving the discontinuity tracking equations (17) associated to the Problem 2, we will obtained $x_r = \frac{1}{2}(x_{r-1}+\sqrt{x_{r-1}^2+4})$ for $r>0$ with the next jump of derivative discontinuities are $\zeta = 0, 1, \frac{1}{2}(1+\sqrt{5}), \frac{1}{4}(1+\sqrt{5}+\sqrt{22+2\sqrt{5}}$. The following abbreviations are defined as follows:

TOL	the prescribe tolerance (TOL = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}).
DTE	the technique of discontinuity tracking equations that has been employed using 1-point implicit method
HMIN	minimum step size.
HMAX	maximum step size.
TS	number of successful steps.
FS	number of failure steps.
FNC	number of function *f* evaluation.
MAXERR	maximum of mixed error test of the computed solution.

Table 1 Comparison for the solution of Problem 1 with and without DTE.

TOL	Technique	HMIN	HMAX	TS	FS	FNC	MAXERR
10^{-2}	Without DTE	2.50E-2	8.00E-1	14	1	39	8.44E-4
	With DTE	1.77E-2	8.00E-1	18	0	48	1.03E-4
10^{-4}	Without DTE	2.50E-3	6.40E-1	33	6	83	3.90E-5
	With DTE	1.77E-3	9.05E-1	28	0	68	1.04E-6
10^{-6}	Without DTE	2.50E-4	5.12E-1	47	10	117	6.93E-6
	With DTE	1.77E-4	7.24E-1	37	0	86	1.04E-8
10^{-8}	Without DTE	2.50E-5	8.19E-1	62	15	154	6.40E-8
	With DTE	1.77E-5	8.19E-1	48	0	108	1.04E-10
10^{-10}	Without DTE	2.50E-6	6.55E-1	86	22	209	3.58E-10
	With DTE	1.77E-6	9.27E-1	58	0	128	1.04E-12

Table 2 Comparison for the solution of Problem 2 with and without DTE.

TOL	Technique	HMIN	HMAX	TS	FS	FNC	MAXERR
10^{-2}	Without DTE	2.50E-2	8.00E-1	18	2	52	3.36E-1
	With DTE	2.73E-2	2.00E-1	16	0	44	4.66E-5
10^{-4}	Without DTE	2.50E-3	6.40E-1	46	10	121	3.46E-1
	With DTE	5.00E-3	8.00E-2	26	0	69	4.25E-6
10^{-6}	Without DTE	1.65E-4	6.78E-1	82	16	225	3.48E-1
	With DTE	5.00E-4	3.20E-2	44	0	116	1.50E-7
10^{-8}	Without DTE	4.81E-6	6.30E-1	144	32	400	3.48E-1
	With DTE	5.00E-5	1.28E-2	78	0	209	2.22E-9
10^{-10}	Without DTE	1.10E-7	9.19E-1	278	38	785	3.48E-1
	With DTE	5.00E-6	5.12E-3	170	0	462	6.56E-12

Table 1 and 2 show the comparison between with and without the strategy of discontinuity tracking equation in 1-point implicit method. In order to avoid the cross of discontinuity points that may lead to the larger number of failure steps, we have restricted the *h* to be included in the mesh points. Here, it can be seen that how important the mechanism of variable step size strategy has been implemented in treating the discontinuity points. Because, once we allow the steps to cross over the discontinuity point, it will produce a larger local truncation error that may not satisfy the condition of $(E_{p,k} \leq TOL)$.

Next, the integration will be restarted just past the discontinuity points that have been detected using the discontinuity tracking equation with the sufficiently small *h*. As the results, it can be observed that the technique of DTE which starts with the minimal step size and increase with the optimal size produces not only better accuracy but it can also give a zero rejected steps. By comparing with the results between Problem 1 and 2, it can be seen that the maximum error with and without DTE has no a big difference in Problem 1 compared to Problem 2. This is actually due to the difficulty and the type of the problem itself where in Problem 1 it is a constant retarded type which is easier compare to the type of time-dependent retarded type. For this case, the results for solving time-dependent retarded type for Problem 2 has shown that the implemented strategy and approach has enhance the smoothness and the accuracy of the method.
As a conclusion, the strategy of discontinuity tracking equation is suitable to be adapted in 1-point implicit method with the mechanism of Runge-Kutta Felhberg step size. The developed algorithm is not only can improve the smoothness of the solution but it has shown the reliability and efficiency in terms of the less number of total steps and function calls in the numerical results.

REFERENCES

[1] Aziz, N.H.A., Majid, Z.A., 2014. Solving Delay Differential Equations of Small and Vanishing Lag Using Multistep Block Method. Journal of Applied Mathematics. Vol. 2014.

[2] Aziz, N.H.A., Majid, Z.A., 2015. The Treatment of Small Delay Case in Linear Multistep Method. Proceedings of the International Conference on Mathematic, Engineering and Industrial Applications, Penang, Malaysia.

[3] Baker, C.T.H., Wille, D.R., 1988. The Propagation of Derivative Discontinuities in Systems of Delay-Differential Equations. Technical Report 160, Dept. of Mathematics, University of Manchester.

[4] Carver, M.B., 1978. Efficient Integration over Discontinuities in Ordinary Differential Equation Simulations. Mathematics and Computers in Simulation, 20(3), 190-196.

[5] Ellison, D., 1981. Efficient Automatic Integration of Ordinary Differential Equations with Discontinuities. Mathematics and Computers in Simulation, 23(1), 12-20.

[6] Enright, W.H., Hayashi, H., 1997. A Delay Differential Equation Solver Based on A Continuous Runge-Kutta Methods with Defect Control. Numerical Algorithms, 16, 349-364.

[7] Fatunla, S.O., 1991. Block Methods for Second Order ODEs. International Journal of Computational Mathematics, 41(1), 55-63.

[8] Gear, C.W., 1971. The Automatic Integration of Ordinary Differential Equations. Communications of the ACM ,14(3), 176-179.

[9] Hairer, E., Norsett, S.P., Wanner, G., 1987. Solving Ordinary Differential Equations I: Nonstiff Problems. Springer Series in Computational Mathematics.

[10] Lenz, S.M., Schloder, J.P., Bock, H.G., 2014. Numerical Computation of Derivatives in Systems of Delay Differential Equations. Mathematics and Computers in Simulation, 96, 124-156.

[11] Li, D., Zhang, C., 2014. L^∞ Error Estimates of Discontinuous Galerkin Methods for Delay Differential Equations. Applied Numerical Mathematics, 82, 1-10.

[12] Majid, Z., Suleiman, M., 2006. 1-Point Implicit Code of Adams Moulton Type to Solve First Order Ordinary Differential Equations. Chiang Mai Journal of Science, 33(2), 153-159.

[13] Neves, K.W., 1975. Automatic Integration of Functional Differential Equations: An Approach. ACM Trans. Math. Soft 1, 357-368.

[14] Paul, C.A.H., 1999. The Treatment of Derivative Discontinuities in Differential Equations. Numerical Analysis Report, 337, 1360-1725.