

## Third derivative integrator for the solution of first order initial value problems

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### Abstract:

Most mathematical models used in physical sciences, biological sciences, medical sciences and engineering are based on Ordinary Differential Equations. Traditionally, solutions to these differential equations can be obtained using analytical methods, however, solutions to certain differential equations are very difficult except the approximate solution by the application of numerical methods. Researchers developed several numerical methods for the solution of ordinary differential equations, but the need to have more accurate numerical method has made it imperative to develop new methods that will yield better results. In this paper therefore, third derivative integrator is developed for solving ordinary differential equations using polynomial approximate solution with the resulted schemes implemented in block. Step and off-step points are considered during the derivation process. The stability properties of the new integrator are established and its accuracy tested on some numerical examples. The results obtained in this study shows that, the new integrator is more efficient for the solution of initial value problems of first order ordinary differential equations, when compared with some existing integrators. The new integrator will be useful for the solution of mathematical problems model in ordinary differential equations.

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### 1. Introduction

Consider the first order initial value problem for ordinary differential equations (ODEs) of the form in equation (1).

$$y' = f(x, y), \quad y(x_0) = y_0, \quad x \in [x_n, x_N] \quad (1)$$

Where:  $f : [x_n, x_N] \times \mathbb{R}^m \rightarrow \mathbb{R}^m$ ,  $y_0 \in \mathbb{R}^m$  is continuous and differentiable.

However,  $f$  is assumed to satisfy the existence and uniqueness theorem [1]. The applications of (1) is vast which includes chemical reactions, control systems, and electronic networks, which lead to systems of differential equations and are difficult to solve because different processes in the system behave with significantly different time scales [1]. Most of the methods for solving differential equations exhibit extreme instability when applied to problems with different time scales and problems with solution components containing widely different time scales are said to be stiff problems [2]. An ordinary differential equation problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results [2].

Block method was first introduced by Milne to generate starting values for predictor-corrector Linear

Multistep Method (LMM) [3] and since then, several block methods has been developed by researchers such as [4 - 13]. According to Lambert [3], hybrid technique was used independently by [14, 15] and later by [16]. The beauty of this method, which was named hybrid methods by [15], is that while retaining certain characteristics of Continuous Linear Multistep Methods (CLMMs), hybrid methods share with Runge-Kutta methods, the property of utilizing data at off-step points and the flexibility of changing step length.

This research work is therefore, concerned with the development of third derivative integrator and considering both step and off-step points for the solution of stiff IVPs ODEs. The new integrator combined the efficiency of single step methods and the high order of accuracy of multistep methods.

### 2. Methodology

Consider the approximate solution in equation (2):

$$y(x) = \sum_{k=0}^4 a_k x^k \quad (2)$$

$$y(a) = y_0, \quad 0 \leq x \leq 1$$

Where:  $x \in [a, b]$ ,  $a_n \in \mathbb{R}$  are the unknown parameters to be determined. The standard collocation

procedure given in equation 3 is used to determine the hybrid point.

$$x_k = a + \frac{(b-a)}{N + \frac{2}{3}} k, \quad k = 0, 1, 2, 3 \quad (3)$$

Evaluating the first, second and third derivatives of equation 2 at  $x = \{x_{n+j} \mid j = 0, \dots, k\}$ , to give the system in equation 4.

$$XA = U \quad (4)$$

Where;

$$A = [a_0, a_1, a_2, a_3, \dots, a_k]$$

$$U = [y_n, y_{n+1}, \dots, y_{n+r}, y_n']^T.$$

Imposing the following conditions

$$\begin{aligned} y(x_{n+j}) &= y_{n+j}, & j &= 0, 1, \dots, r \\ y'(x_{n+j}) &= f_{n+j}, & j &= 0, 1, \dots, s \\ y''(x_{n+j}) &= g_{n+j}, & j &= 0, 1, \dots, \tau \\ y'''(x_{n+j}) &= l_{n+j}, & j &= 0, 1, \dots, q \end{aligned}$$

on equation 2, gives

$$X = \begin{bmatrix} 1 & x_n & x_n^2 & \cdots & x_n^k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n+r} & x_{n+r}^2 & \cdots & x_{n+r}^k \\ 0 & 1 & 2x_n & \cdots & kx_n^{k-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 2x_{n+s} & \cdots & kx_{n+s}^{k-1} \end{bmatrix}$$

$$B_0(t) = -\frac{1}{22044960} t \begin{pmatrix} 181258560t - 848073240t^2 \\ +2506236390t^3 - 4904760168t^4 \\ +6459882660t^5 - 5672136360t^6 \\ +3186833265t^7 - 1037168440t^8 \\ +148811124t^9 - 22044960 \end{pmatrix}$$

$$B_{\frac{3}{11}}(t) = -\frac{14641}{2006581248} t^2 \begin{pmatrix} -120784608t + 526417542t^2 \\ -1319277456t^3 + 2062354140t^4 \\ -2052361344t^5 + 1267941213t^6 \\ -444383632t^7 + 67641420t^8 \\ +12492144 \end{pmatrix}$$

$$B_{\frac{6}{11}}(t) = -\frac{14641}{218700000} t^2 \begin{pmatrix} -22054680t + 108403110t^2 \\ -308192040t^3 + 542058660t^4 \\ -599196840t^5 + 405788625t^6 \\ -154023320t^7 + 25123956t^8 \\ +2099520 \end{pmatrix}$$

$$B_{\frac{9}{11}}(t) = -\frac{14641}{352719360} t^2 \begin{pmatrix} -64139040t + 317355570t^2 \\ -919504656t^3 + 1669922100t^4 \\ -1926513600t^5 + 1371415815t^6 \\ -549330320t^7 + 94697988t^8 \\ +6123600 \end{pmatrix}$$

Where:  $k = r + s + \tau$ .

Solving equation 4 for the unknown parameters using Cramer's rule and substitute the results into equation 2 gives

$$y_{n+t} = \sum_{j=0}^r \alpha_j(t) y_{n+j} + h \sum_{j=0}^s \beta_j(t) f_{n+j} + h^2 \sum_{j=0}^{\tau} \gamma_j(t) g_{n+j} \quad (5)$$

Where:  $\alpha_j(t)$ ,  $\beta_j(t)$ , and  $\gamma_j(t)$  are polynomial of degree

$$r + s + \tau - 1 \text{ and } t = \frac{x - x_n}{h}.$$

Evaluating the first, second and third derivatives of equation (2) at

$$[x_n, x_{n+\frac{3}{11}}, x_{n+\frac{6}{11}}, x_{n+\frac{9}{11}}, x_{n+1}],$$

$$[x_{n+\frac{3}{11}}, x_{n+\frac{6}{11}}, x_{n+\frac{9}{11}}, x_{n+1}] \text{ and } x_{n+1}$$

Respectively to give continuous scheme shown in equation (6):

$$\begin{aligned} y_{n+t} &= A_0(t)y_n + B_0(t)f_n + B_{\frac{3}{11}}(t)f_{n+\frac{3}{11}} + \\ &B_{\frac{6}{11}}(t)f_{n+\frac{6}{11}} + B_{\frac{9}{11}}(t)f_{n+\frac{9}{11}} + \beta_1(t)f_{n+1} + \\ &C_{\frac{3}{11}}(t)g_{n+\frac{3}{11}} + C_{\frac{6}{11}}(t)g_{n+\frac{6}{11}} + C_{\frac{9}{11}}(t)g_{n+\frac{9}{11}} + \\ &C_1(t)g_{n+1} + D_1(t)l_{n+1} \end{aligned} \quad (6)$$

Where;  $A_0(t) = y(t)$

$$B_1(t) = \frac{1}{409600000} t^2 \begin{pmatrix} -2071994243040t + 9988048879830t^2 \\ -28118354703120t^3 + 49539513673980t^4 \\ -55424375867520t^5 + 38292614947125t^6 \\ -14910578290960t^7 + 2503903058668t^8 \\ +202386904560 \end{pmatrix}$$

$$C_{\frac{3}{11}}(t) - \frac{1331}{418037760} t^2 \begin{pmatrix} -31298400t + 125947710t^2 \\ -298883088t^3 + 449179500t^4 \\ -433973760t^5 + 262040625t^6 \\ -90188560t^7 + 13528284t^8 \\ +3674160 \end{pmatrix}$$

$$C_{\frac{6}{11}}(t) - \frac{1331}{17010000} t^2 \begin{pmatrix} -5964840t + 27134730t^2 \\ -71590680t^3 + 117697580t^4 \\ -122660120t^5 + 78961575t^6 \\ -28696360t^7 + 4509428t^8 \\ +612360 \end{pmatrix}$$

$$C_{\frac{9}{11}}(t) - \frac{1331}{19595520} t^2 \begin{pmatrix} -12428640t + 59279850t^2 \\ -164814048t^3 + 286278300t^4 \\ -315316320t^5 + 214244415t^6 \\ -81989600t^7 + 13528284t^8 \\ +1224720 \end{pmatrix}$$

$$C_1(t) - \frac{1}{107520000} t^2 \begin{pmatrix} -45589793760t + 220435430670t^2 \\ -622847277360t^3 + 1102071898620t^4 \\ -1239073260480t^5 + 860806248225t^6 \\ -337215025840t^7 + 56994660492t^8 \\ +4442059440 \end{pmatrix}$$

$$D_1(t) \frac{1}{32256000} t^2 \begin{pmatrix} -340472160t + 1652810670t^2 \\ -4692718800t^3 + 8351301420t^4 \\ -9452868480t^5 + 6618098025t^6 \\ -2615468240t^7 + 446433372t^8 \\ +33067440 \end{pmatrix}$$

Evaluating the continuous scheme (6) at  $t = \frac{3}{11}, \frac{6}{11}, \frac{9}{11}, 1$  to give the discrete schemes as follows

$$y_{n+\frac{3}{11}} = \begin{pmatrix} y_n + \frac{7751459}{147581280} hf_n - \frac{4002699}{10092544} hf_{n+\frac{3}{11}} \\ - \frac{772767}{1100000} hf_{n+\frac{6}{11}} - \frac{2305777}{1774080} hf_{n+\frac{9}{11}} \\ + \frac{15706153166067}{5996953600000} hf_{n+1} - \frac{6106533}{69386240} h^2 g_{n+\frac{3}{11}} \\ - \frac{2322129}{8470000} h^2 g_{n+\frac{6}{11}} - \frac{484321}{1084160} h^2 g_{n+\frac{9}{11}} \\ - \frac{114493174461}{524733440000} h^2 g_{n+1} + \frac{282781287}{52473344000} h^3 l_{n+1} \end{pmatrix} \quad (7)$$

$$y_{n+\frac{6}{11}} = \begin{pmatrix} y_n + \frac{242831}{4611915} hf_n - \frac{8331}{28672} hf_{n+\frac{3}{11}} \\ - \frac{20349}{34375} hf_{n+\frac{6}{11}} - \frac{73723}{55440} hf_{n+\frac{9}{11}} \\ + \frac{506951470449}{187404800000} hf_{n+1} - \frac{183207}{2168320} h^2 g_{n+\frac{3}{11}} \\ - \frac{14136}{48125} h^2 g_{n+\frac{6}{11}} - \frac{15679}{33880} h^2 g_{n+\frac{9}{11}} \\ - \frac{3692926647}{16397920000} h^2 g_{n+1} + \frac{9113229}{1639792000} h^3 l_{n+1} \end{pmatrix} \quad (8)$$

$$y_{n+\frac{9}{11}} = \begin{pmatrix} y_n + \frac{863691}{16397920} h f_n - \frac{2905227}{10092544} h f_{n+\frac{3}{11}} \\ - \frac{517023}{1100000} h f_{n+\frac{6}{11}} - \frac{241833}{197120} h f_{n+\frac{9}{11}} \\ + \frac{16492954164723}{5996953600000} h f_{n+1} - \frac{5849253}{69386240} h^2 g_{n+\frac{3}{11}} \\ - \frac{2436561}{8470000} h^2 g_{n+\frac{6}{11}} - \frac{516321}{1084160} h^2 g_{n+\frac{9}{11}} \\ - \frac{119979360189}{524733440000} h^2 g_{n+1} + \frac{295658343}{52473344000} h^3 l_{n+1} \end{pmatrix} \quad (9)$$

$$y_{n+1} = \begin{pmatrix} y_n + \frac{1161169}{22044960} h f_n - \frac{577133579}{2006581248} h f_{n+\frac{3}{11}} \\ - \frac{102355231}{218700000} h f_{n+\frac{6}{11}} - \frac{401997937}{352719360} h f_{n+\frac{9}{11}} \\ + \frac{1164359523}{409600000} h f_{n+1} - \frac{35232901}{418037760} h^2 g_{n+\frac{3}{11}} \\ - \frac{4888763}{17010000} h^2 g_{n+\frac{6}{11}} - \frac{9265091}{19595520} h^2 g_{n+\frac{9}{11}} \\ - \frac{24940007}{107520000} h^2 g_{n+1} + \frac{183247}{32256000} h^3 l_{n+1} \end{pmatrix} \quad (10)$$

Writing equations 7, 8, 9 and 10 in block, we have

$$A^{(1)} Y_{m+1} = \begin{bmatrix} A^{(0)} Y_m + h B^{(0)} F_m + h B^{(1)} F_{m+1} \\ + h^2 \gamma^{(1)} G_{m+1} + h^3 \Gamma^{(1)} L_{m+1} \end{bmatrix} \quad (11)$$

Where:

$$Y_{m+1} = \begin{bmatrix} y_{n+\frac{3}{11}}, y_{n+\frac{6}{11}}, y_{n+\frac{9}{11}}, y_{n+1} \end{bmatrix}^T,$$

$$Y_m = \begin{bmatrix} y_{n-1}, y_{n-2}, y_{n-3}, y_n \end{bmatrix}^T,$$

$$F_m = \begin{bmatrix} f_{n-1}, f_{n-2}, f_{n-3}, f_n \end{bmatrix}^T,$$

$$F_{m+1} = \begin{bmatrix} f_{n+\frac{3}{11}}, f_{n+\frac{6}{11}}, f_{n+\frac{9}{11}}, f_{n+1} \end{bmatrix}^T,$$

$$G_{m+1} = \begin{bmatrix} g_{n+\frac{3}{11}}, g_{n+\frac{6}{11}}, g_{n+\frac{9}{11}}, g_{n+1} \end{bmatrix}^T,$$

$$L_{m+1} = \begin{bmatrix} l_{n-1}, l_{n-2}, l_{n-3}, l_{n+1} \end{bmatrix}^T,$$

$$A^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad A^{(0)} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad B^{(0)} = \begin{bmatrix} 0 & 0 & 0 & \frac{7751459}{147581280} \\ 0 & 0 & 0 & \frac{242831}{4611915} \\ 0 & 0 & 0 & \frac{863691}{16397920} \\ 0 & 0 & 0 & \frac{1161169}{22044960} \end{bmatrix},$$

$$B^{(1)} = \begin{bmatrix} \frac{4002699}{10092544} & \frac{772767}{1100000} & \frac{2305777}{1774080} & \frac{15706153166067}{5996953600000} \\ \frac{8331}{28672} & \frac{20349}{34375} & \frac{73723}{55440} & \frac{506951470449}{187404800000} \\ \frac{2905227}{517023} & \frac{517023}{241833} & \frac{241833}{16492954164723} & \frac{16492954164723}{5996953600000} \\ \frac{10092544}{577133579} & \frac{1100000}{102355231} & \frac{197120}{401997937} & \frac{5996953600000}{1164359523} \\ \frac{2006581248}{218700000} & \frac{218700000}{352719360} & \frac{352719360}{409600000} & \frac{409600000}{409600000} \end{bmatrix},$$

$$\gamma^{(1)} = \begin{bmatrix} \frac{6106533}{69386240} & \frac{2322129}{8470000} & \frac{484321}{1084160} & \frac{114493174461}{524733440000} \\ \frac{183207}{2168320} & \frac{14136}{48125} & \frac{15679}{33880} & \frac{3692926647}{16397920000} \\ \frac{5849253}{2436561} & \frac{2436561}{516321} & \frac{516321}{119979360189} & \frac{119979360189}{524733440000} \\ \frac{69386240}{35232901} & \frac{8470000}{4888763} & \frac{1084160}{9265091} & \frac{524733440000}{24940007} \\ \frac{418037760}{17010000} & \frac{17010000}{19595520} & \frac{19595520}{107520000} & \frac{107520000}{107520000} \end{bmatrix}$$

and

$$\Gamma^{(1)} = \begin{bmatrix} 0 & 0 & 0 & \frac{282781287}{52473344000} \\ 0 & 0 & 0 & \frac{1639792000}{295658343} \\ 0 & 0 & 0 & \frac{52473344000}{183247} \\ 0 & 0 & 0 & \frac{32256000}{183247} \end{bmatrix}$$

## 2.1 Stability analysis

### 2.1.1 Order and error constant of the Method

Evaluating each row of equation (5) in a Taylor series about

$x_n$  gives [8].

$$L[y(x); h] = y_{n+t} - \sum_{j=0}^r \alpha_j(t) y_{n+j} - h \sum_{j=0}^s \beta_j(t) f_{n+j} \quad (12)$$

$$h^{p+n} \neq 0$$

$$p + n = 11$$

Where:  $n$  is the order of the differential equation. Therefore, the order of the integrator developed are

$$p = [10, 10, 10, 10]^T \text{ with error constant}$$

$$\left[ -\frac{55311633}{5624063651084032000} h^{11}, -\frac{1764207}{175751989096376000} h^{11}, -\frac{56728593}{5624063651084032000} h^{11}, -\frac{7787}{771436866816000} h^{11} \right]^T \quad (13)$$

#### 2.1.1.1 Consistency of the Method

The order of the integrator is  $p = 10 > 1$ , therefore, the integrator is consistent [8, 9].

### 2.1.2 Zero Stability of the Block Method

The block integrator (11) is zero stable since the roots  $z_s, s = 1, 2, 3, \dots, n$  of the first characteristics polynomial  $\rho(\lambda)$  is defined by

$$\rho(\lambda) = \det[A^{(1)}\lambda - A^{(0)}] = 0 \quad (14)$$

$$\lambda^4 - \lambda^3 = \lambda^3(\lambda - 1) = 0$$

Solving for  $\lambda$  we have  $\lambda = [0, 0, 0, 1]^T$ . Hence the block integrator (11) is zero stable [8, 9].

#### 2.1.2.1 Convergence

Since the integrator is consistent and zero-stable, therefore, it is convergent [8].

### 2.1.3 Region of Absolute Stability

This is achieved by substituting the test equation

$$y' = \lambda y \quad (15)$$

In the block integrator. This gives the region of absolute stability as seen in Figure 1,

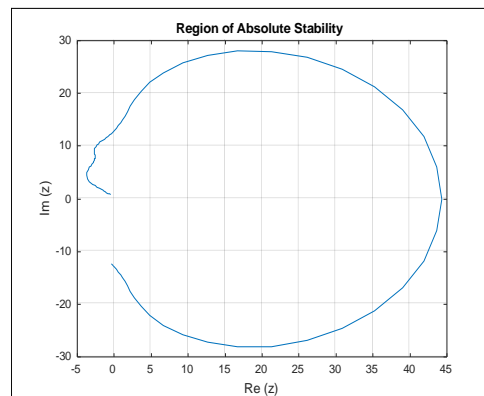


Figure 1: Region of absolute stability of 3DI

## 3. Numerical examples

Table 1 show the abbreviation used in this section and their meaning.

Table 1: Notations	
Abbreviation	Meaning
3DI	Third Derivative Integrator
OMOP	One-Step Method with Two off-step point
OMTOP	One-Step Method with Two off-step Point
3BEBDF	3 Point Block Extended Backward Differential Formula
3BBDF	3 Point Block Backward Differential Formula

The following examples are considered to test the efficiency of the new integrators.

Example 1:

$$y' = -y \quad y(0) = 1, \quad h = 0.1, \quad 0 \leq x \leq 1$$

with exact solution: [12]

$$y(x) = \exp(-x)$$

Table 2 show the absolute error of the result of example 1 and that in [12].

Table 2: Result of example 1:

$x$	3DI	OMOP in [12]	OMTOP in [12]
0.1	2.3456263 (-8)	1.2574666 (-8)	4.4204169 (-7)
0.2	4.433356 (-8)	2.2756058 (-8)	7.999513 (-7)
0.3	2.5314111 (-9)	3.0885799	1.0857388 (-6)
0.4	2.9627122 (-9)	3.726217 (-8)	1.3098892 (-6)
0.5	3.7258142 (-9)	4.2145258 (-8)	1.4815455 (-6)
0.6	4.7145121 (-9)	4.5761528 (-8)	1.608669 (-6)
0.7	5.8793099 (-9)	4.8307866 (-8)	1.698189 (-6)
0.8	6.274953 (-9)	4.995516 (-8)	1.756088 (-6)
0.9	3.867419 (-9)	5.0851416 (-8)	4.420417 (-7)
1.0	4.433714 (-9)	5.1124784 (-8)	7.999513 (-7)

Example 2:

$$y_1' = -1002y_1 + 1000y_2^2 \quad y_1(0) = 1$$

$$y_2' = y_1 - y_2(1 + y_2(x)) \quad y_2(0) = 1$$

with exact solution: [13]

$$y(x) = \begin{bmatrix} \exp(-2x) \\ \exp(-x) \end{bmatrix}$$

Table 3 show the maximum error of the result of example 2 and that in [11] and [13].

Table 3: Result of example 2

$x$	Max (Error) in 3DI	Max (Error) in [11]	Max (Error) in [13]
0.1	5.1204 (-09)	3.2221 (-04)	1.9470 (-05)
0.2	4.9715 (-09)	2.4712 (-04)	2.22106 (-05)
0.3	4.9978 (-09)	1.4958 (-04)	1.7065 (-06)
0.4	5.1332 (-09)	9.3454 (-05)	8.3233 (-06)
0.5	5.8221 (-09)	5.7570 (-05)	3.1284 (-06)
0.6	6.0127 (-09)	1.0152 (-05)	2.1172 (-07)
0.7	6.4215 (-09)	1.0606 (-06)	7.6218 (-08)
0.8	2.3344 (-10)	5.5600 (-07)	1.8354 (-08)
0.9	2.5521 (-10)	2.35600 (-07)	3.2536 (-08)
1.0	3.2330 (-10)	1.5270 (-07)	7.6541 (-09)

Example 3

$$y_1' = -y_1 + 95y_2 \quad y_1(0) = 1 \quad 0 \leq x \leq 10$$

$$y_2' = -y_1 - 97y_2 \quad y_2(0) = 1$$

with exact solution

$$y(x) = \frac{1}{47} \begin{bmatrix} 95e^{-2x} - 48e^{-96x} \\ 48e^{-96x} - e^{-2x} \end{bmatrix}$$

the eigenvalues are  $-2$  and  $-96$ . [12]

Table 4 show the absolute error of the result of example 3 and that in [12].

Table 4: Result of example 3

$x$	3DI	3BEBDE in [12]	3BBDE in [12]
0.02	5.87601e-003	3.06562e-002	1.14619e-002
0.03	6.39566e-003	3.93978e-002	6.89917e-002
0.04	4.14259e-004	8.39129e-003	1.05286e-002
0.05	7.31353e-004	9.02719e-004	1.07915e-003
0.06	5.01462e-005	9.09318e-002	1.08172e-004

## 4. Discussions of results

The results obtained in Table 2 to Table 4 clearly show that, the new block integrator performed better than the results obtained by the existing methods in [11], [12] and [13] respectively. These established that the new integrator compete effectively with the existing methods with better approximation.

## 5. Conclusions

Third derivative integrator is developed while considering step and off-step points. Polynomial approximate solution is considered and the resulted integrators implemented in block. The stability properties of the new block integrator are established and found to be of order 10, stable, consistent and convergent with large region of absolute stability as seen in Fig. 1. The efficiency of the integrator is tested on some numerical examples which connote that, the new block integrator is efficient for the solution of initial value problems of first order ordinary differential equations.

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