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Continuous Approach for Deriving Self-Starting Multistep Methods for Initial Value Problems in Ordinary Differential Equations

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Abstract: This study presents a continuous approach for the derivation of self-starting multistep methods for the numerical treatment of ordinary differential equations. The popular k-step Adams Moulton class requires single step methods to obtain the (k-1) starting values. In this paper we consider a collocation approach at the various interpolation points to obtain a set of k-multistep methods. The set of methods are of uniform order and A-stable. Two examples are presented here.

Key words: Self-starting multistep methods, legendre polynomial and functions, kerturbation term, convergence, block methods, hybrid methods

INTRODUCTION

Consider the initial value problem

$$y'(x) = f(x,y(x)); \quad y(0) = y_0; \quad y_0 \in R^n \qquad (1.1)$$

Classical multistep methods to solve the ivp (1.1) are the basis of some important codes for non-stiff differential equations as discussed in many texts such as Dahlquist and Bjorck, 1974; Fatunla, 1989; Hairer *et al*., 1996; Onumanyi *et al*., 1999. The general k-step method is written as

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=o}^{k} \beta_j f_{n+j} \qquad \alpha_k \neq 0 \qquad (1.2)$$

where , . = 0 are real parameters, . . 0, . .+. >0 whenever . = 0 in (1.2), the method is said to be explicit otherwise it is implicit. Explicit multistep algorithms based on rigid frames were proposed by Crouch and Grossman in Lambert (1991). For an application of (1.2), we require a starting procedure to compute the approximates *y, y, ..., y* to *y(x+h), y(x+2h), ..., y((x+(k-1)h)*. This has been the standard approach to implement multistep methods. All computer codes will have to integrate as a subroutine codes for single step methods like the Runge-Kutta methods. Butcher (1975), introduced the concept of multistep Runge-Kutta methods. In contrast to single-step methods, where numerical solution is obtained solely from the differential equation and the initial condition, to implement these methods, there are three basic ways of obtaining the initial starting values at each stage of the iteration: using the Taylor series expansion of the exact solution, using any single step method such as Runge-Kutta methods, or using a low-order Adams methods. The motivation for this paper is the possibility of evolving a numerical approach that will circumvent the conventional search for single step or lower ordered methods to obtain starting values. The negative effects of the other methods used might divert the trajectory towards instability. The idea is to get self-starting multistep methods that will preserve both its initial accuracy and stability properties. Generally, to implement the multistep methods (1.2) most users resort to single step methods. These are methods which use only one starting value at each step. The most popular of this class is the Runge-Kutta methods.

Let s be an integer and a, a, ..., a, a, ..., ab, ..., b, c, ..., c be real coefficients. Then the method

y = y+h(bk+...+bk) (1.3)

is called an s -stage Explicit Runge-Kutta method (ERK) for ivp(1.1)where the ki's for (i = 1, 2, ..., s) are defined as:

k = f(x, y); k = f(x+ch, y+hakk = f(x+ch, y+h(ak+ak...,;
k = f(x+ch, y+hak+...+as,s-ks-))

Usually, the ci satisfy the conditions

$$c_i = \sum_{j=1}^{i-1} a_{ij} \qquad (1.4)$$

In general, let bi, aij(i, j = 1, ..., s) be real numbers and let $c_i = \sum_{j=1}^{s} a_{ij}$ then an s-stage Runge-Kutta method is given by

$$k_i = f(t_0 + c_i h,\ y_0 + h\sum_{j=1}^{s} a_{ij}k_j);\quad y_1 = y_0 + h\sum_{i=1}^{s} b_i k_i \qquad (1.5)$$

whenever a = 0, for i j; we have (1.3) i.e. ERK and if a = 0, for i < j and at least one a 0, we have a diagonal implicit Runge-Kutta method. If all diagonal elements are identical, a= , for i = 1, ..., s), then (1.5) becomes a singly diagonal implicit Runge-Kutta method. In all other cases, (1.5) is called an implicit Runge-Kutta method.

In the past few decades, the desire to make the advantages of multistep methods accessible to single step methods in particular Runge-Kutta methods led to many well known approaches in literature such as the generalised multistep methods of Gragg and Stetter, modified multistep methods of Butcher *et al.* (1975, 1980), the hybrid methods of Gear in Dahlquist and Bajorck, 1974 and the parallel methods of Fatunla (1989).

A GENERAL INTEGRATION PROCEDURE

Consider the system

$$y' = f(x, y);\quad y(x_0) = y_0 \qquad (2.1)$$

where f satisfies the Lipschitz condition of the existence and uniqueness of solution. Let the general linear methods be represented as

$$U = SU + h(x, u, h) \qquad (2.2)$$

where S is a square matrix and is an m×n matrix. Let m be the dimension of the differential Eq. 2.1, q m be the dimension of the difference Eq. 2.2 and x = x+nh be the subdivision points of an equidistant grid.

The Integration procedure can be splited into three parts:

- A forward step procedure. S is independent of (2.1).
- A correct value function z(x, h), which gives an interpretation of the values U; z = z(x, h) is to be approximated by u. It is assumed that the exact solution y(x) of (2.1) can be recovered from z(x, h).
- A starting procedure (h), which specifies the starting value u = (h), (h) z = z(x, h). The discrete problem arising from (3.10) is given by

U = SU+h (x, u, h); n = 0, 1, 2, ...; U = (h) (2.3)

RESULTS

In this section we discuss the two examples of the new continuous collocation approaches to formulate self-starting multistep methods. These are

- Block Hybrid Using Simpson Interpolant with continuous formulation
- The power series collocation method.

Example one: The new block hybrid method using the simpson interpolant: Consider the continuous collocation approximate to the ivp (1.1)

$$y(x) = \sum_{i=1}^{t} \alpha_i(x) y_{n+1} + \sum_{i=1}^{s} h_n \beta_i f_{n+i} \qquad (3.1)$$

where n = 0, k, 2k, ..., j; t and s denotes the number of interpolation and collocation points respectively, h is the variable step-size. and x x• x where

$$\begin{aligned} a_i(x) &= \sum_{r=1}^{t} C_{r1}\phi_r(x) + \sum_{r=t+1}^{p} C_{r1}\phi_r(x) \quad \text{and} \\ h_n\beta_i(x) &= \sum_{r=1}^{t} C_{r1}\phi_r(x) + \sum_{r=t+1}^{p} C_{r1}\phi_r(x) \end{aligned} \qquad (3.2)$$

C are elements of the inverse matrix C.

Let Y (x) = a (x)+a (x)+...+a (x); x x x (3.3)

Imposing the following conditions

$$\left.\begin{aligned} a_1\phi_1(x_j) + a_2\phi_2(x_j) + \ldots + a_p\phi_p(x_j) = y_j; \quad j = 1,2,\ldots,t \\ a_1\phi_1'(x_i) + a_2\phi_2'(x_i) + \ldots + a_p\phi_p'(x_i) = f_i; \quad i = 1,2,\ldots,s \end{aligned}\right\} \qquad (3.4)$$

Let $\underline{a} = (a_1, a_2, \ldots, a_p)^T;\quad \phi = (\phi_1, \phi_2, \ldots, \phi_p)^T;$
$\underline{F} = (y_{n+1}, \ldots, y_{n+t}, f_{n+1}, \ldots, f_{n+s})^T$

$$\underline{D} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & . & . & . & \phi_p(x_1) \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \phi_1(x_t) & \phi_2(x_t) & . & . & . & \phi_p(x_t) \\ \phi_1(c_1) & \phi_2(c_1) & . & . & . & \phi_p(c_1) \\ . & . & . & . & . & . \\ \phi_1(c_s) & \phi_2(c_s) & . & . & . & \phi_p(c_s) \end{bmatrix} \qquad (3.5)$$

We then have

$$\underline{Da} = \underline{F} \Rightarrow \underline{a} = \underline{D^{-1}F} = \underline{\underline{C}}\underline{F} \Rightarrow \underline{\underline{C}} = \underline{D^{-1}} \qquad (3.6)$$

Rewriting (4.3) as matrix multiplication of the form

$$\begin{aligned} Y(x) &= (a_1, a_2, \ldots, a_p)^T.(\phi_1, \phi_2, \ldots, \phi_p)^T = \underline{a}^T \phi(x) = (\underline{\underline{CF}})^T \phi(x). \\ &= (y_{n+1}, \ldots, y_{n+t}, f_{n+1}, \ldots, f_{n+s})(C_{ij})\phi_1(x), \ldots, \phi_t \\ &\quad (x), \phi_{t+1}(x), \ldots, \phi_{t+s}(x))^T \end{aligned} \tag{3.7}$$

where

$$Cij = \begin{bmatrix} c_{11} & c_{12} & \cdot\cdot\cdot & c_{t1} & c_{t+1,1} & \cdot\cdot\cdot & c_{t+s,1} \\ c_{12} & c_{22} & \cdot\cdot\cdot & c_{t2} & c_{t+1,2} & \cdot\cdot\cdot & c_{t+s,2} \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ c_{1t} & c_{2t} & \cdot\cdot\cdot & c_{tt} & c_{t+1,t} & \cdot\cdot\cdot & c_{t+s,t} \\ c_{1,t+1} & c_{2,t+1} & \cdot\cdot\cdot & c_{t,t+1} & c_{t+1,t+1} & \cdot\cdot\cdot & c_{t+s,t+1} \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ \cdot & \cdot & \cdot\cdot\cdot & \cdot & \cdot & \cdot\cdot\cdot & \cdot \\ c_{1,t+s} & c_{2,t+s} & \cdot\cdot\cdot & c_{t,t+s} & c_{t+1,t+s} & \cdot\cdot\cdot & c_{t+s,t+s} \end{bmatrix} \tag{3.8}$$

Substituting back into (3.8) into (3.7) yields the following continuous scheme:

$$Y(x) = \sum_{i=1}^{t} \tau_i(x) y_{n+i} + h_n \sum_{i=1}^{s} \psi_i f_{n+i} \tag{3.9}$$

where

$$\tau_i(x) = \sum_{r=1}^{t} C_{ri}\phi_r(x) + \sum_{r=t+1}^{p} C_{ri}\phi_r(x) \tag{3.10}$$

$$\psi_i(x) = \sum_{r=1}^{t} \frac{C_{ri}}{h_n}\phi_r(x) + \sum_{r=t+1}^{p} \frac{C_{ri}}{h_n}\phi_r(x) \tag{3.11}$$

which is equivalent to

$$Y(x) = \sum_{i=0}^{t+m-1}\left[\sum_{j=0}^{t-1} C_{i+1,j+1} y_{n+j} + \sum_{j=0}^{m-1} C_{i+1,j+t+1} f_{n+j}\right] x^i \tag{3.12}$$

We consider a particular case with the following parameters:

k = 2; t = 1; m = k+2;
I , (x, x); $(\overline{x_0} = x_n; \overline{x_1} = x_{n+1}; \overline{x_{\frac{3}{2}}} = x_{n+\frac{3}{2}}; \overline{x_2} = x_{n+2})$

Putting these parameters and follow through the algorithm described above, we obtain the following continuous scheme:

$$\begin{aligned} y(x) = y_n &+ \begin{bmatrix} -\frac{1}{12h^3}(x - x_n)^4 + \frac{1}{2h^2}(x - x_n)^3 \\ -\frac{13}{12h}(x - x_n)^2 + (x - x_n) \end{bmatrix} f_n + \\ &\left[\frac{1}{2h^3}(x - x_n)^4 - \frac{7}{3h^2}(x - x_n)^3 + \frac{3}{h}(x - x_n)^2\right] f_{n+1} + \\ &\frac{1}{3h}\left[-\frac{2}{h^2}(x - x_n)^4 + \frac{8}{h}(x - x_n)^3 - 8\left((x - x_n)^2\right)\right] f_{n+\frac{3}{2}} + \\ &\left[\frac{1}{4h^3}(x - x_n)^4 - \frac{5}{6h^2}(x - x_n)^3 + \frac{3}{4h}(x - x_n)^2\right] f_{n+2} \end{aligned} \tag{3.13}$$

Collocating (3.13) at the points x = x.; x = x3. and x = x. we obtain the following three discrete schemes which is the new Block Hybrid method:

$$y_{n+1} = y_n + \tfrac{h}{6}[2f_n + 7f_{n+1} - 4f_{n+\frac{3}{2}} + f_{n+2} \tag{3.14}$$

$$y_{n+\frac{3}{2}} = y_n + \tfrac{3h}{64}[7f_n + 30f_{n+1} - 8f_{n+\frac{3}{2}} + 3f_{n+2} \tag{3.15}$$

$$y_{n+2} = y_n + \tfrac{h}{3}[f_n + 4f_{n+1} + f_{n+2}] \tag{3.16}$$

Note that (3.16) is the recovered h/3 Simpson's method which is both a maximal and optimal multistep method Dahlquist (1974). Going through the standard analysis for multistep methods, the three methods are of uniform order four. The Table 1 shows the respective error constants of the methods.

Stability analysis: We verify using the root condition of the first characteristic polynomial of the hybrid block method

$$\rho(R) = \det\left[\sum_{i=0}^{k} A^i R^{k-1}\right] \Rightarrow \det\left[RA^0 - A^1\right] \tag{3.17}$$

Solving (3.17) for R, we have that $R_j \leq 1$, j = 1,2,3. Hence the method is zero stable. Since it is of uniform order greater than 1, it is consistent, therefore it is convergent.
Using the stability function

$$M(z) = B_2 + ZA_2(I - ZA_1)^{-1}B_1 \tag{3.18}$$

Table 1: The standard analysis for multistep methods, the three methods are of uniform order four

Method	Error constant
(3.14)	$-\frac{31}{2880}$
(3.15)	$-\frac{51}{5120}$
(3.16)	$\frac{-1}{90}$

where A and B are the partitioned matrices for the block system:

$$\begin{bmatrix} Y \\ y_{i+1} \end{bmatrix} = \begin{bmatrix} A_1 & | & B_1 \\ - & - & - \\ A_2 & | & B_2 \end{bmatrix} \begin{bmatrix} hf(y) \\ y_{i-1} \end{bmatrix} \qquad (3.19)$$

we obtain the following matrix equation:

$$\begin{bmatrix} y_n \\ y_{n+1} \\ y_{n+\frac{3}{2}} \\ y_{n+2} \\ ---- \\ y_{n+2} \\ y_{n+1} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & | & 0 & 1 \\ \frac{2}{6} & \frac{7}{6} & \frac{-4}{6} & \frac{1}{6} & | & 0 & 1 \\ \frac{21}{64} & \frac{90}{64} & \frac{-24}{64} & \frac{9}{64} & | & 0 & 1 \\ \frac{1}{3} & \frac{4}{3} & 0 & \frac{1}{3} & | & 0 & 1 \\ - & - & - & - & - & - & - \\ \frac{1}{3} & \frac{4}{3} & 0 & \frac{1}{3} & | & 0 & 1 \\ \frac{2}{6} & \frac{7}{6} & \frac{-4}{6} & \frac{1}{6} & | & 0 & 12 \end{bmatrix} \begin{bmatrix} f_n \\ f_{n+1} \\ f_{n+\frac{3}{2}} \\ f_{n+2} \\ --- \\ f_{n+1} \\ f_n \end{bmatrix} \qquad (3.20)$$

By obtaining the stability polynomial .(,.) = det(.I-m(.)) through the substitution of the matrices A, A, B and B into (3.18) and resolving it , it becomes obvious that the block method is A stable.

Example two: the power series collocation method: The power series approach earlier described in the earlier work of the author Fato Kun, 2004 is used as the basis for collocation approximation with the Legendre Polynomials as the perturbation term. The Legendre function is transformed from [-1,1] into [x, x.]. The exact solution of the perturbed form for the equation (1.1) is given by

$$y_k(x) = \sum_{j=0}^{k} a_j Q_j(k) \qquad x \in [x_n, x_{n+k}], \qquad k > 0 \quad (3.21)$$

where Qj(x) = x; . 0 is the power series. If we subject equation(3.20) to the constraints

$$\bar{y}(x_{n+j}) = y_{n+j}; \qquad j = 0,1,2,...,k-1 \qquad (3.22)$$

and the following collocation equations

$$\bar{y}'(x_{n+k}) = f_{n+k}; \quad \text{and} \quad \bar{y}'(x_{n+k-1}) = f_{n+k-1} \qquad (3.23)$$

In addition we use the .- parameter as the perturbation term defined as

$$\sum_{j=0}^{k} a_j Q_j(x) = f(x,y) + \tau P_k(x) \qquad (3.24)$$

where P.(x) is the Legendre polynomial of degree k and valid in x.x.x. and . is a parameter to be determined.

Table 2: The conventional analysis on order and error constants of the schemes (3.26)-(3.30)

Method	Error constant
(3.26)	$\frac{-1}{56}$
(3.27)	$\frac{-1}{32}$
(3.28)	$\frac{-1}{93}$
(3.29)	$\frac{-79}{12500}$
(3.30)	$\frac{-1}{73}$

For a particular k = 5 in (3.21)-(3.24), we the continuous scheme as follows:

$$\bar{y}(x) = y_{n+4} + (x^5 - x^5_{n+4})a_5 + (x^4 - x^4_{n+4})a_4 + (x^3 - x^3_{n+4})a_3 + (x^2 - x^2_{n+4})a_2 + (x - x_{n+4})a_1 \qquad (3.25)$$

Collocating (3.25) at the following grid points x, x., x., x. and x. we obtain the following system of discrete schemes:

$$y_n - y_{n+4} = \frac{-2h}{9\varepsilon} \begin{Bmatrix} \zeta_1 k_6 + \zeta_2 k_5 + \zeta_3 k_4 \\ +\zeta_4 k_3 + \zeta_5 k_2 + \zeta_6 k_1 \end{Bmatrix} \qquad (3.26)$$

$$y_{n+1} - y_{n+4} = \frac{-h}{\varepsilon} \begin{Bmatrix} \eta_1 k_6 + \eta_2 k_5 + \eta_3 k_4 \\ +\eta_4 k_3 + \eta_5 k_2 - \eta_6 k_1 \end{Bmatrix} \qquad (3.27)$$

$$y_{n+2} - y_{n+4} = \frac{-h}{9\varepsilon} \begin{Bmatrix} \delta_1 k_6 - \delta_2 k_5 - \delta_3 k_4 \\ -\delta_4 k_3 - \delta_5 k_2 + \delta_6 k_1 \end{Bmatrix} \qquad (3.28)$$

$$y_{n+3} - y_{n+4} = \frac{-h}{9\varepsilon} \begin{Bmatrix} \gamma_1 k_6 - \gamma_2 k_5 - \gamma_3 k_4 \\ +\gamma_4 k_3 - \gamma_5 k_2 + \gamma_6 k_1 \end{Bmatrix} \qquad (3.29)$$

$$y_{n+5} - y_{n+4} = \frac{h}{54\varepsilon} \begin{Bmatrix} \rho_1 k_6 + \rho_2 k_5 - \rho_3 k_4 \\ +\rho_4 k_3 - \rho_5 k_2 + \rho_6 k_1 \end{Bmatrix} \qquad (3.30)$$

Where
. =1680 and the *k's* are the derivative functions, while the coefficients of *k's* are as given below:

.=137;.=1667;.=12122;.=2662;.=11437;.=2215;.=21;.= 462; .=2352; .=1302; .=987; .=84; .=5; .=4897; .=20782; .=4082; .=647; .=163; .=188; .=6211; .=11686; .=3664; .=1286; .=211;.=31161; .=83721; .=37914; .=18006; .=4719; .=465.

Following the conventional analysis on order and error constants of the schemes (3.26)-(3.30), we obtain the following results in Table 2:

IMPLEMENTATION PROCEDURE

The methods of examples (1) and (2) are implemented as parallel methods for accurate and fast process of numerical integration. Since each of the methods are implicit, at every stage, the values of the approximates (y, y ..., y of the previous iteration serves as automatic predictors for the new stage in the integration. Thus the block of these schemes can be implemented simultaneously without seeking for any single step scheme.

CONCLUSION

Two major examples of self starting multistep methods by collocating the continouos methods have been presented. The resulting methods are analysed for accuracy, stability and convergence. Implementation is to be done via parallel computing. The methods are expected to be well suited for stiff differential equations because of the A-stablity property. Work is ongoing in the aspect of introducing hybrid points in example Two particularly using the Gauss points hence arriving at Radau-like methods but with better anticipated results.

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