A Continuous linear Multistep Method for Improved Performance in the Solutions of first order System of Ordinary Differential Equations

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Abstract
In this paper we develop a generalized derivation formula for the construction of a continuous linear multistep method (clmm) for solving first order system of ordinary differential equations (ODE's). It is based on interpolation and collocation leading to a formula that involves a matrix inverse and an arbitrary basis vector function. This is done to widen the scope of application of the new approach. A global error estimation of the approximate method id described. The clmms have more ability to solve the ODE's than the conventional discrete ones (lmms). For a fixed order and mesh-size the initial value problem (IVP) can be solved without looking for any other method to start the integration process over sub-intervals, which do not overlap. The method applies uniformly and directly to the two-point boundary-value problem (BVP).

1. Introduction and Notations

The derivation of Imms through interpolation and collocation (see Lambert ((1973, 1991), Lie and Norsett (1989) and our earlier works in Onumanyi et al (1994), 1999, 2001)) is now well known. Atkinson (1989) describes collocation as probably now the most important numerical procedure for obtaining continuous methods for ODE's.

In section 2 of this paper a general framework is presented for the construction of clmms/Imms through interpolation and collocation. This is based on a matrix inverse and an arbitrary basis vector function for the ODE's of the form.

$$Ly = \frac{dy(x)}{dx} = f(x,y), a \le x \le b; \qquad 1.1$$

Where y satisfies initial or boundary conditions. The analytic solution y is assumed to exist and unique in $[a,b]$. The k-step approximate method we seek.

$$y(x) = u(x), \quad a \le x \le b$$

Has the form

$$u(x) = \sum_{v=0}^{i-1} \phi_v(x) y_{n+v} + h \sum_{v=0}^{m-1} \psi_v(x) f_{n+v} \qquad 1.2$$

Where h = x_{n+1} - x_n is a constant step-size, n = 0, 1… $N = \frac{(b-a)}{h}$, t, $(0 < t \le k-1)$ denotes the number of interpolation points, m > 0 denotes the number of distinct collocation points.

$$\phi_V(x) = \sum_{I=0}^{t+m-1} \phi_{i+1,\,v} P_i(x), \qquad V \in \{0, 1, ..., t-1\} \tag{1.3}$$

$$h\psi_v(x) = \sum_{i=0}^{i+m-1} h\psi_{i+1,\,v} P_i(x), \quad v = 0, 1, ..., m-1 \tag{1.4}$$

The constants $\phi_{i+1,v}$ *and* $h\psi_{i+1,\,v}$ are underdetermined elements of the following (t + m) x (t+m) dimensional matrix.

$$C = . \begin{bmatrix} \phi_{1,0} & \phi_{1,1} & \cdots & \phi_{1,t-1} & h\psi_{1,0} & \ldots h\psi_{1,m-1} \\ \phi_{2,0} & \phi_{2,1} & \cdots & \phi_{2,t-1} & h\psi_{2,,0} & \ldots h\psi_{2,m-1} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \phi_{i+1,0} & \phi_{i+1,1} & \cdots & \phi_{1i+1,t-1} & h\psi_{1,0} & \ldots h\psi_{i+1,m-1} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \phi_{t+m,0} & \phi_{i+m,1} & \cdots & \phi_{1i+m,t-1} & h\psi_{1t+m,0} & \ldots h\psi_{i+m,m-1} \end{bmatrix} \tag{1.5}$$

Where i = 0, 1, …, t + m-1 in (1.5)

We define the following

$$\underline{a} = (a_0, a_1, ..., a_{t+m-1})^T \tag{1.6}$$

$$\underline{V} = (y_n, y_{n+1}, ..., y_{n+t-1}, f_n, f_{n+1}, ..., f_{n+m-1})^T \tag{1.7}$$

$$\underline{P}(x) = (P_0(x), P_1(x), ..., P_{t+m-1}(x))^T \tag{1.8}$$

Denotes an arbitrary basis function and

$$M = \begin{bmatrix} P_o(x_n) & ..... & P_{i+m-1}(x_n) \\ P_o(x_{n+1}) & ..... & P_{i+m-1}(x_{n+1}) \\ . & & . \\ . & & . \\ . & & . \\ P_o(x_{n+t-1}) & ..... & P_{t+m-1}(x_{n+t-1}) \\ LP_o(\bar{x}_0) & .... & LP_{t+m-1}(\bar{x}_0) \\ LPo(xn+1) & .... & LP_{t+m-1}(\bar{x}_1) \\ . & & . \\ . & & . \\ . & & . \\ LP_0(\bar{x}_{m-1}) & .... & LP_{t+m-1}(\bar{x}_{m-1}) \end{bmatrix} \quad 1.9$$

The resulting piecewise continuous (polynomial or non-polynomial) approximate solution U(x) obtained in section 2 has a large link to many classes of numerical methods for the first order system (1.1). We showed in Onumanyi et al (1994, 1999) that on the same fixed meshes for the class of Adams Moulton methods the higher order members could be applied successively by choosing different values of the step number. This desirable feature of the proposed approach leads to obtaining good global error estimation and hence cheap step-size control strategy for an automatic program or software for its implementation (though this practical aspects is not done in this paper).

Finally, in section 3, we consider some applications of the clmms obtained in section 2. The continuous form has more ability to solve the ODE's than the discrete ones. The initial-value problem (IVP) is solved, for instance, without looking for any other methods to start the integration process. Moreover, if desired the whole integration can be achieved with one matrix difference equation over sub-intervals which do not overlap (Jennings (1987), p. 59 and Lambert (1991), p. 53). In this way, the proposed approach applies uniformly and directly to the two-point boundary-value problem (BVP)

2. Derivation

We state the main result of this section as follows.

Theorem (2.1)

Let U(x) satisfy the interpolation and collocation conditions, respectively of the form.

i. $U(x_{n+j}) = y_{n+j}, j \in \{0,1,...,t-1\}$

ii. $LU(\bar{x}_j) = f_{n+j}, j = 0,1,...,m-1$

Where the non-singular matrix M is defined by (1.9) and C is defined by (1.5).

Then (a)

$$U(x) = \underline{V}^T (M^{-1})^T \underline{P}(x) \qquad (b) \quad C = M^{-1}. \qquad 2.0$$

Proof of theorem (2.1)

(a) Consider (1.2), (1.3) and (1.4) to obtain

$$U(x)=\sum_{i=0}^{t+m-1}\left\{\sum_{v=0}^{t-1}\phi_{i+1,v}y_{n+v}+\sum_{v=0}^{m-1}h\psi_{i+1,v}f_{n+v}\right\}P_i(x) \qquad 2.1$$

$$=\sum a_iP_i(x) \qquad 2.2$$

Where

$$a_i=\sum_{v=0}^{t-1}\phi_{i+1,v}y_{n+v}+\sum_{v=0}^{m-1}h\psi_{i+1,v}f_{n+v} \qquad i=0,1,\dots,t+m-1 \qquad 2.3$$

a_{ir} are $t+m$ undetermined constants. Now consider (2.2) in a vector form

$$U(x)=\underline{a}^T\,\underline{P}(x) \qquad 2.4$$

By imposing the conditions (i) and (ii) in the theorem (2.1) on (2.4) lead to the system

$$M\,\underline{a}=\underline{V} \qquad 2.5$$

Thus

$$\underline{a}=M^{-1}\underline{V} \qquad 2.6$$

From (2.6), (2.4) becomes

$$U(x)=\underline{V}^T(M^{-1})^T\,\underline{P}(x) \qquad 2.7$$

Which proves (a) part of the theorem (2.1)

(b) We can write (2.3) in a vector form

$$a_i=(\phi_{i+1,0},\dots,\phi_{i+1,t-1},h\psi_{i+1,0},\dots,h\psi_{i+1,m-1})\underline{V}$$
$$i=0,1,\dots,t+m-1. \qquad 2.8$$

From (1.5) , (2.8) becomes

$$a_i=\underline{C}_{i+1}\underline{V},\quad i=0,1,\dots t+m-1 \qquad 2.9$$

where $\underline{C}_i$ denotes (i+1)th row of the matrix C in (1.5). Hence (2.9) can be put in the form

$$\underline{a}^T=(C\underline{V})^T \text{ or } (\underline{a}=C\underline{V}) \qquad 2.10$$

Comparing (2.6) and (2.10) we obtain the result $C = M^{-1}$ of the (b) part of the theorem (2.1) and this completes the proof of the theorem (2.1).
We remark that (2.7) under no circumstances should be used as a numerical integrator because of the cost in obtaining M^{-1} at each step of the integration process. Rather it is a generalized derivation procedure for the next section.

3. Specification of Methods and Applications Arising from (2.7) and C= M^{-1}.

The formula (2.7) with $C = M^{-1}$ has a unifying focus for the derivation of many known classes of clmms by choosing the appropriate parameters involved in the formula.

2.0

These include the Adams methods, the Backward Differentiation formulae and the Trapezoidal rule method based on a special exponential basis.

b. The Adams Methods

For the numerical solution of the nonstiff IVP this sub-class of clmms can be derived by the following parameter selection in (2.7). WE consider $\{P_i(x) = x^i,\ i = 0,1,...,t+m-1;\ t = 1;\ m = 1;\ m = k$ (explicit), $m = k+1$ (implicit) with collocation points $X_n, X_{n+1},..., X_{n+k}$; the interpolation point is X_{n+k-t}; and $\underline{V} = (y_{n+k-1}, f_n, f_{n+1},..., f_{n+k-1}, f_{n+k})^I\}$.

We give the first and second members of the implicit case, i.e. the continuous Adams-Moulton methods, for the scaled variable $\tau = (x - x_{n+k=1})/h, -(k-1) \le \tau \le 1$ where $\tau = 1$ Corresponds to $x = x_{n+k}$, the point at which the coefficients of the discrete methods are recovered.

$k = 1; 0 \le \tau \le 1,\ x_n \le x \le x_{n+1}$

$$U(\tau) = y_n + h\left(\tau \frac{1}{2}\tau^2\right)f_n + h\left(\frac{1}{2}\tau^2\right)f_{n+1}$$

$$U(\tau = 1) \equiv y_{n+1} = y_n + \frac{h}{2}(f_n + f_{n+1}) \qquad \text{(Trapezoidal rule)}$$

$K = 2;\ -1 \le \tau \le 1, x_n \le x \le x_{n+2}$

$$U(\tau) = y_{n+1} + h\left(\frac{-3}{12}\tau^2 + \frac{2}{12}\tau^3\right)f_n + h\left(\tau - \frac{4}{12}\tau^3\right)f_{n+1} + h\left(\frac{3}{12}\tau^2 + \frac{2}{12}\tau^3\right)f_{n+2}$$

$$U(\tau = 1) \equiv y_{n+2} = y_{n+1} + \frac{h}{12}(-f_n + 8f_{n+1} + 5f_{n+2}) \qquad \text{i}$$

$$U(\tau = 1) \equiv y_{n+2} = y_{n+1} + \frac{h}{12}(-f_n + 8f_{n+1} + 5f_{n+2})$$

This last equation can be written as

$$y_n = y_{n+1} - \frac{h}{12}(-f_{n+2} + 8f_{n+1} + 5f_n) \qquad \text{ii}$$

Where (i) and (ii) can be combined as simultaneous numerical integrators for the (ODEs). They constitute the same integrator in forward (i) and backward (ii) directions respectively. The order is 3 with error constant $\left(\frac{-1}{24}, \frac{1}{24}\right)^T$ and absolute stability interval (-6,0).

The block method consisting of (i) and (ii) is zero-stable as we can easily show as follow.

Transferring all the unknowns y_{n+1} and y_{n+2} in (i) and (ii) to the left hand side and normalizing the equations we have in matrix form.

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} y_{q+1} = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} y_q + h\left[\begin{pmatrix} \frac{8}{12} & \frac{-1}{12} \\ \frac{16}{12} & \frac{4}{12} \end{pmatrix} f_{q+1} + \begin{pmatrix} 0 & \frac{5}{12} \\ 0 & \frac{4}{12} \end{pmatrix} f_q\right] \qquad 3.1$$

Where $y_{q+1} = (y_{n+1}, y_{n+2})^I$,

$$y_q = (y_{n-1}, y_n)^I, q = 0,1,2,3,..., n = 0,2,4,6,...$$

Setting $h=0$ in (3.1), we obtain the zero-stability polynomial in a parameter R as follows

$$P(R) = \left| R\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \right| = (R-1).$$

Thus from $R(R=1)=0$ gives $R=0$ or $R=0$ or $R=1$.

Therefore the block method (3.1) is zero-stable and being of order 3 (consistent) implies it is convergent.

For $n=0, q=o, (y_1, y_2)^T$ are obtained simultaneously from the value y over the sub-interval $|x_0, x_2|$.

For $n=2, q=1, (y_3, y_4)^T$ are obtained simultaneously from the previous block values $(y_1, y_2)^T$ over the sub-interval $\|x_2, x_4\|$, and so on. This way the sub-intervals do not over-lap. The same block method (3.1) can save the IVP and the BVP directly without requiring any other one-step method to obtain y_1 separately from (3.1). If desired (3.1) can be used only for this purpose and then return to the single use of (i) over sub-intervals $[x_0, x_2], [x_1, x_3], [x_2, x_4]$, and so on which overlap each other in the conventional way. On the other hand, the use of (3.1) over sub-intervals, which do not overlap in one matrix difference equation, can directly solve both the IVP and BVP (see Onumanyi et al. (1999))

b. The Backward Differentiation Formulae (BDF)

Here, we consider the following parameters in (2.7) for the stiff ODEs {Pi (x) = x^i, i=0, 1, …, t+m-1; t = k with x_n, x_{n+1}, … x_{n+k-1} as the interpolation points; x_{n+k} (implicit) as the only collocation point and V = (y_n, y_{n+1}, … y_{n+k-1}, f_{n+k}). The first and second members of the BDF class are stated as follows;

$K = 1;\ 0 \le \tau \le 1;\ x_n \le x \le_{xn+1}$

$U(\tau) = y_n + h\tau f_{n+1}$

$U(\tau = 1) = y_n + hf_{n+1}$ (Backward Euler Method) $U(\tau = 1) = y_{n+1}$

$K = 2;\ -1 \le t \le 1;\ x\ xn \le x \le x_{n+2}$

$$U(\tau) = \left(\frac{-2}{3}\tau + \frac{1}{3}\tau\right)y_n + \left(1 + \frac{2}{3}\tau - \frac{1}{3}\tau^2\right)y_{n+1} + h\left(\frac{1}{3}\tau + \frac{1}{3}\tau^2\right)f_{n+1}$$

$$U(\tau=1) = \frac{-1}{3}y_n + \frac{4}{3}y_{n+1} + \frac{2}{3}hf_{n+2}(U(\tau=1) = y_{n+2})$$

From the first derivative values

$$\frac{du}{dt}(t=0) = h\frac{du}{dx}(x = x_{n+1}) = hf_{n+1}$$

We obtain a second equation of the form

$$\frac{-1}{3}y_n + \frac{2}{3}y_{n+1} = h\left(f_{n+1} \quad \frac{-1}{3}f_{n+2}\right) \quad \text{(iv)}$$

The combination of (i) and (ii) form the normalized block method given as follows

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} y_{q+1} = \begin{pmatrix} 0 & -2 \\ 0 & \frac{-1}{3} \end{pmatrix} y_q + h\begin{pmatrix} \frac{3}{2} & -2 \\ 2 & 0 \end{pmatrix} f_{q+1} \quad 3.3$$

It can be easily shown to be zero-stable. The members are each of order two and hence the integrator (3.3) is of order two with an error constant $\left(\frac{-2}{9},\ \frac{-5}{18}\right)^T$. both members of (3.3) are A-stable hence (3.3) is A-stable and thus suitable for stiff systems. Its implementation follows the description above for the Adams-Moulton method.

(c) The Trapezoidal Method based on Exponential basis functions

In this example the parameters of the trapezoidal method are the same but in (2.7) the basis in replaced from $P_i(x) = x^i, i = 0,1,2$ to a new one.

$P_0(x) = e^{\lambda_1 x}, P_1(x) - r^{\lambda_1^* x}, P_2(x) = e^{\lambda_2 x},$

Where the constants λ_1, $\lambda 1$, λ_2 are eigenvalues of the given system of ODEs and λ_1. λ_1 are complex conjugates, λ_2 is a real number.

Then $\underline{V} = (y_n, f_n, f_{n+1})$ for the Trapezoidal method, and the matrix M in (1.9) becomes

$$M = \begin{bmatrix} e^{\lambda_1 x_n} & e^{\lambda^*{}_1 x_n} & e^{\lambda_2 xLn} \\ \lambda_1 e^{\lambda_1 x_n} & \lambda_1^* e^{\lambda_1^* x_n} & \lambda_2 e^{\lambda_2 x_n} \\ \lambda_1 e^{\lambda_1 x_{n+1}} & \lambda_1^* e^{\lambda_1 x_{n+1}} & \lambda_2 e^{\lambda_1 x_{n+1}} \end{bmatrix} \qquad 3.4$$

With $C = M^{-1}$, the resulting approximate solution is given by (2.7) which can be evaluated at $x = x_{n+1}$ to give an order three method of the form

$$y_{n+1} - y_n = R\, f_n + S\, f_{n+1} \qquad 3.5$$

Where the real constants *Q, R, S* are defined as follows:

$$Q = \frac{1}{\sigma}\left[(\lambda^*{}_1\lambda_2)(e^{\lambda_2 h} - e^{\lambda^* h})e^{\lambda_1 h} + (-\lambda_1\lambda_2)(e^{\lambda_3 h} - e^{\lambda_1^* h} + (\lambda_1\lambda_1^*(e^{\lambda_1^* h} - e^{\lambda_1 h})e^{\lambda_1 h}\right] \qquad 3.6$$

$$R = \frac{1}{\sigma}\left[(\lambda_2 e^{\lambda_1 h} - \lambda_1 e^{\lambda_1^* h} - (\lambda_2 e^{\lambda_2 h} - \lambda_1^* e^{\lambda^*{}_1 h})e^{\lambda_1 h} + (\lambda_1 e^{\lambda_1 h} - \lambda_1^* e^{\lambda_1 h})e^{\lambda_1 h}\right] \qquad 3.7$$

$$S = \frac{1}{\sigma}\left[(\lambda_2 - \lambda_1^*)e^{\lambda_1 h} + (\lambda_1 - \lambda_2)e^{\lambda_1^* h} + (\lambda_1^* - \lambda_1)e^{\lambda_2 h}\right] \qquad 3.8$$

$$\sigma = (\lambda_1^*\lambda_2)(e^{\lambda_2 h} - e^{\lambda_1^* h}) - (\lambda_1\lambda_2)(e^{\lambda_1 h} - e^{\lambda_1 h}) + \qquad 3.9$$
$$+ (\lambda_1\lambda_1^*)(e^{\lambda_1^* h} - e^{\lambda_1 h})$$

We show that the one-step discrete method consisting of (3.5)-(3.9) is L-stable, whereas the conventional Trapezoidal method is A-stable but not L-stable. We state this result in the Theorem (3.1):

Theorem 3.1

The integrator formula (3.5) is L-stable if either

(I) $R > 0, \quad p \neq 0$

(ii) $R.Q, \quad$ p > -1

(iii) $R > -Q, \quad p < +1$

Proof of Theorem (3.1)
Consider the test scalar equation

$y^{i} = \lambda, \quad \operatorname{Re}\lambda < 0$

The single root of the stability polynomial for the integrator formula is given by

$$r = (P + Qh\lambda)/(1 = Rh\lambda)$$
$$|r| = \left|\frac{(P + Qh\lambda)}{(-Rh\lambda}\right| < 1$$
$$-1 < \frac{P + Qh\lambda}{1 - Rh\lambda}, < 1$$
$$-1 + Rh\lambda \quad P + Qh\lambda \ < 1 - Rh\lambda$$

$1 - Rh\lambda \ > 0,$ for any Q and $P \neq 0$

Thus,

(i) $\quad 1 - Rh\lambda > 0 \Rightarrow h\lambda < \frac{1}{\mathrm{R}} \Rightarrow$ A - stable if $R > 0, \ P \neq 0$

(ii) $\quad -1 + Rh\lambda < P + Qh\lambda \Rightarrow (R - Q)h\lambda < (1 + P)$

$\quad \Rightarrow h\lambda < \frac{1 + P}{R + Q} \Rightarrow$ A - stable if $R > Q, P > 1$

(iii) $\quad P + Qh\lambda < 1 - Rh\lambda \Rightarrow (R + Q)h\lambda < (1 - P)$

$\quad \Rightarrow h\lambda < \frac{1 - P}{R + Q} \Rightarrow$ A - stable if $R > -Q, P < 1$

The application of the numerical integration to the test scalar equation yields.

$$\frac{y_{n+1}}{y_n} = \frac{P + \lambda Q}{1 - \lambda R} \tag{3.10}$$

The values of $\lambda_1 = \lambda, \ \lambda_1^* = 0$ and $\lambda_2 = 0$ yield

$P(\lambda, \lambda_1^* = 0, \lambda_2 = 0) = 1 \ \forall$ values of λ^* including $\lambda_1^* = 0$ a

$Q(\lambda, \lambda_1^* = 0, \lambda_2 = 0) = \left[\frac{-1 = e^{h\lambda} - h\lambda e^{h\lambda}}{\lambda - \lambda e^{h\lambda}}\right]$ by L'Hospital rule b

$Q(\lambda, \lambda_1^* = 0, \lambda_2 = 0) = \left[\frac{1 = e^{h\lambda} - e^{h\lambda}}{\lambda - \lambda e^{h\lambda}}\right]$ by L'Hospital rule c

Substituting (a), (b), (c) into (3.10) we obtain

$$\frac{P + \lambda\,\mathrm{Q}}{1 - \lambda\, R} = \frac{\left\{1 + \frac{\lambda\left[-1 + (1 - h\lambda)e^{\lambda h}\right]}{\left[\lambda - \lambda e^{h\lambda}\right]}\right\}}{\left\{1 - \frac{\lambda\left[1 + \mathrm{h}\lambda - e^{\lambda h}\right]}{\lambda - \lambda e^{h\lambda}}\right\}}$$
$$= \frac{\lambda - \lambda^{h\lambda} - \lambda + \lambda\, e^{h\lambda} - h\lambda^{\,2}\ e^{h\lambda}}{\lambda - \lambda\, e^{h\lambda} - \lambda - h\lambda^2 + \lambda\, e^{h\lambda}}$$
$$= e^{h\lambda}$$

$$\lim_{Re(h\lambda)\to-\infty}\left[\frac{P+\lambda Q}{1-\lambda R}\right]=\lim_{Re(h\lambda)\to-\infty}\left[e^{\lambda h}\right]\to e^{-\infty}=\frac{1}{e^{\infty}}=0.$$

This shows a correct asymptotic behaviour of the numerical integrator. Therefore if (i) or (ii) or (iii) holds then the method is L-stable. This implies that for very stiff IVP or highly oscillatory IVP, this method should succeed where the conventional trapezoidal rule method fails.

4. Conclusion

A unified approach to the derivation of continuous linear multistep methods (elms) with an arbitrary basis function has been presented. The approach unifies into a single formula, which is based on a matrix inverse through interpolation and collocation, many classes of methods that have in the past been derived by various procedures. Now the same continuous method and its first derivative function (if necessary) provide simultaneous discrete methods that can treat both the IVP and BVP uniformly and directly with a single matrix difference equation. This eliminates the need for any other method to provide starting values for the IVP for a fixed order and fixed order and fixed mesh-size. For the IVP as well as the BVP it eliminates overlap of successive sub-interval (see Onumanyi et al (2001)).

Finally, we hope to investigate other basis functions in a future paper. These include rational functions for singularity treatment, chebyshev polynomials for uniform accuracy across the integration interval and special basis for delay problems (see Rubin Qu (1997)), while many more can be constructed as new problems arise.

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