

A Functionally Fitted Linear Multistep Method

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1 Introduction

Consider the k -step linear multistep method with variable coefficients

$$\begin{aligned} y_{n+k} + \alpha_{k-1}y_{n+k-1} + \cdots + \alpha_0y_n \\ = h(\beta_k(t_n, h)f_{n+k} + \beta_{k-1}(t_n, h)f_{n+k-1} + \cdots + \beta_0(t_n, h)f_n), \end{aligned} \quad (1)$$

$$f_j = f(t_j, y_j), \quad t_j = t_0 + jh, \quad j = 0, 1, \dots,$$

for solving the initial value problem

$$y'(t) = f(t, y), \quad y(t_0) = y_0, \quad t \in [t_0, T]. \quad (2)$$

In the method (1) the coefficients α 's are constant, while β 's are the functions of t and h . We assume that the method is consistent and zero-stable, i.e, the first characteristic polynomial given by

$$\rho(\zeta) = \alpha_k\zeta^k + \alpha_{k-1}\zeta^{k-1} + \cdots + \alpha_0, \quad \alpha_k = 1, \quad (3)$$

has root $\zeta = 1$, which is usually labeled by ζ_1 , and all the other roots ζ_l ($l = 2, \dots, k$) satisfy

$$|\zeta_i| \leq 1, \quad i = 2, \dots, k,$$

and if $|\zeta_i| = 1$ then ζ_i is simple.

2 Functionally Fitted Linear Multistep Method

In this paper we assume that the solution of (1) is approximated by the linear combination of some functions. In order to fit the method to this approximated solution, for given α 's we determine β 's by the system of the equations

$$\begin{aligned} \alpha_k\Phi_m(t+kh) + \alpha_{k-1}\Phi_m(t+(k-1)h) + \cdots + \alpha_0\Phi_m(t) \\ = h(\beta_k\varphi_m(t+kh) + \beta_{k-1}\varphi_m(t+(k-1)h) + \cdots + \beta_0\varphi_m(t)), \\ m = 1, 2, \dots, k+1, \end{aligned} \quad (4)$$

where $\varphi_m(t)$ ($m = 1, 2, \dots, k+1$) are analytic functions on $[t_0, T]$, and

$$\Phi_m(t) = \int_{t_0}^t \varphi_m(\tau) d\tau, \quad m = 1, 2, \dots, k+1.$$

Here we define the polynomial, the second characteristic polynomial, by

$$\sigma(\zeta) = \beta_k\zeta^k + \beta_{k-1}\zeta^{k-1} + \cdots + \beta_0. \quad (5)$$

Using the polynomial, equation (4) can be expressed by

$$\rho(\Delta) \Phi_m(t) = h \sigma(\Delta) \varphi_m(t), \quad m = 1, 2, \dots, k+1, \quad (6)$$

where Δ is the shift operator defined by

$$\Delta^j \Phi(t) = \Phi(t + jh), \quad j = 0, 1, \dots$$

The method (1) with the coefficients given by (4) or (6) integrates the equation (2) exactly, if its solution is expressed by a linear combination of $\{\Phi_m(t)\}_{m=1}^{k+1}$. Here we call the method *functionally fitted linear multistep* (FLM) method. Here we give the theorem for the uniqueness and the analyticity of β 's.

Theorem 1 *Let the base functions $\{\varphi_m(t)\}_{m=1}^{k+1}$ be analytic on $[t_0, T]$, and let the Wronskian matrix $W(\varphi_1(t), \varphi_2(t), \dots, \varphi_{k+1}(t))$ given by*

$$W = \begin{pmatrix} \varphi_1(t) & \varphi_2(t) & \cdots & \varphi_{k+1}(t) \\ \varphi_1^{(1)}(t) & \varphi_2^{(1)}(t) & \cdots & \varphi_{k+1}^{(1)}(t) \\ \vdots & \vdots & \cdots & \vdots \\ \varphi_1^{(k)}(t) & \varphi_2^{(k)}(t) & \cdots & \varphi_{k+1}^{(k)}(t) \end{pmatrix} \quad (7)$$

be nonsingular on that interval. Then the $\beta_j(t, h)$ given by (6) are unique and analytic at $h = 0$.

Proof Equation (6) can be rewritten as

$$C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1}) \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} = h^{-1} \rho(\Delta) \begin{pmatrix} \Phi_1(t) \\ \Phi_2(t) \\ \vdots \\ \Phi_{k+1}(t) \end{pmatrix}, \quad (8)$$

where C is the Casoratian matrix given by

$$C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1}) \equiv \begin{pmatrix} \varphi_1(t) & \varphi_1(t+h) & \cdots & \varphi_1(t+kh) \\ \varphi_2(t) & \varphi_2(t+h) & \cdots & \varphi_2(t+kh) \\ \vdots & \vdots & \cdots & \vdots \\ \varphi_{k+1}(t) & \varphi_{k+1}(t+h) & \cdots & \varphi_{k+1}(t+kh) \end{pmatrix}. \quad (9)$$

For the uniqueness of β_j we show the non-singularity of C . The Casoratian matrix C is

related to the Wronskian matrix W by the formula

$$\begin{aligned}
C &= W^T \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & h & 2h & \cdots & kh \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & h^k/k! & (2h)^k/k! & \cdots & (kh)^k/k! \end{pmatrix} + O(h^{k+1}) \\
&= W^T \begin{pmatrix} 1 & & & & \\ & h & & & \\ & & h^2/2 & & \\ & & & \ddots & \\ & & & & h^k/k! \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 2 & \cdots & k \\ 0 & 1 & 2^2 & \cdots & k^2 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 1 & 2^k & \cdots & k^k \end{pmatrix} + O(h^{k+1}),
\end{aligned} \tag{10}$$

since $\varphi_m(t)$ are analytic by assumption. If we use the convention that $0^0 = 1$, then the third matrix in the right-hand side is nothing but the Vandermonde matrix associated with $0, 1, \dots, k$, so we denote it by $V(0, 1, \dots, k)$. We have from (10)

$$\det C = \det W \left(\prod_{j=0}^k \frac{1}{j!} \right) \det V(0, 1, \dots, k) h^{\frac{k(k+1)}{2}} + O(h^{\frac{k(k+1)}{2}+1}). \tag{11}$$

The uniqueness and analyticity for $h > 0$ follows from the non-singularity of $V(0, 1, \dots, k)$.

Next we show the uniqueness and analyticity of β_j at $h = 0$. By Cramer's rule we have

$$\beta_j = \frac{\det C_j}{\det C}, \quad j = 0, 1, \dots, k, \tag{12}$$

where

$$C_j = \begin{pmatrix} \varphi_1(t) & \cdots & \frac{1}{h} \rho(\Delta) \Phi_1(t) & \cdots & \varphi_1(t + kh) \\ \varphi_2(t) & \cdots & \frac{1}{h} \rho(\Delta) \Phi_2(t) & \cdots & \varphi_2(t + kh) \\ \vdots & \cdots & \vdots & \cdots & \vdots \\ \varphi_{k+1}(t) & \cdots & \frac{1}{h} \rho(\Delta) \Phi_{k+1}(t) & \cdots & \varphi_{k+1}(t + kh) \end{pmatrix}.$$

Each of the entries of the $(j+1)$ st column of the matrix is given by

$$h^{-1} \rho(\Delta) \Phi_m(t) = \sum_{l=0}^{\infty} \mu_l \left(\frac{h^l}{l!} \varphi_m^{(l)}(t) \right), \quad m = 1, 2, \dots, k+1, \tag{13}$$

where

$$\mu_l = \frac{1}{l+1} \sum_{j=0}^k \alpha_j j^{l+1}.$$

Therefore we have for C_j

$$C_j = W^T \cdot \text{diag}(1, h, h^2/2, \dots, h^k/k!) \cdot V_j + O(h^{k+1}), \tag{14}$$

where

$$V_j = \begin{pmatrix} & & & & j+1 & & \\ 1 & 1 & \cdots & \mu_0 & \cdots & 1 & \\ 0 & 1 & \cdots & \mu_1 & \cdots & k & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ 0 & 1 & \cdots & \mu_k & \cdots & k^k & \end{pmatrix},$$

which leads to

$$\det C_j = \det W \det V_j \left(\prod_{l=0}^k \frac{1}{l!} \right) h^{\frac{k(k+1)}{2}} + O(h^{\frac{k(k+1)}{2}+1}). \quad (15)$$

We can find from (11) and (15) that $\det C$ and $\det C_j$ have common zero, that is $h = 0$, and that the orders of the zero of $\det C_j$ is higher or equal to that of $\det C$ since $\det V \neq 0$. This means that the singularity of β_j at $h = 0$ is removal. Therefore $\beta_j(t, h)$ is analytic and unique even at $h = 0$, if we define

$$\beta_j(t, 0) = \det V_j / \det V, \quad j = 0, \dots, k. \quad \blacksquare$$

Next we consider the accuracy of the FLM for the case that the solution of (2) cannot be expressed exactly by the linear combination of $\{\Phi_m(t)\}_{m=1}^{k+1}$. As is the case of constant coefficient methods, we consider the local error

$$e_{n+k} = y_{n+k} - y(t_{n+k}),$$

under the so-called localizing assumption that

$$y_{n+j} = y(t_{n+j}), \quad j = 0, 1, \dots, k-1.$$

As for the case of constant coefficient methods, if

$$e_{n+k} = y_{n+k} - y(t_{n+k}) = O(h^{p+1}), \quad h \rightarrow 0 \quad (16)$$

then we call the *method is of order p*. Note that in this case we must consider the behaviors of the error in the situation that the coefficients of the FLM are being changed as functions of h , when $h \rightarrow 0$.

In order to consider the local error we associate with the method the difference operator

$$\begin{aligned} \mathcal{L}[y(t); h] &= \sum_{j=0}^k \alpha_j y(t+jh) - h \sum_{j=0}^k \beta_j(t, h) y'(t+jh), \\ &= \rho(\Delta) y(t) - h\sigma(\Delta) y'(t). \end{aligned} \quad (17)$$

Using the operator we have

$$e_{n+k} = \left(1 - h \beta_k(t_n, h) \frac{\partial f}{\partial y} \right)^{-1} \mathcal{L}[y(t_n); h].$$

From (22) we have $K = 0$ since W is nonsingular by assumption. For the q th column of K , this means

$$C_q^{(l)} = 0, \quad l = 0, 1, \dots, k+1-q, \quad q = 1, 2, \dots, k+1,$$

which leads to

$$C_q = O(h^{k+2-q}), \quad q = 1, 2, \dots, k+1, \quad (23)$$

unless the higher order terms, $C_q^{(k+2-q)}$, $C_q^{(k+3-q)}$, \dots , happen to be 0. Therefore for sufficiently smooth function $y(t)$, the operator $\mathcal{L}[y(t); h]$ is of order at least $k+1$. ■

From $C_q^{(0)} = 0$ ($q = 1, 2, \dots, k+1$), we have

$$\sum_{j=0}^k \beta_j^{(0)} j^{q-1} = \frac{1}{q} \sum_{j=0}^k j^q \alpha_j, \quad q = 1, 2, \dots, k+1, \quad (24)$$

which determines $\beta_j^{(0)}$ uniquely, and the resulting values are, of course, independent of $\{\varphi_m(t)\}_{m=1}^{k+1}$. Thus we have:

Corollary 1 *The constant terms $\beta_j^{(0)}$, which are independent of $\{\varphi_m(t)\}_{m=1}^{k+1}$, are uniquely determined, and the attainable order of the LM method with $(\alpha_j, \beta_j^{(0)})$ is $k+1$ or $k+2$, when the step number k is odd or even, respectively, since the method is a zero-stable method (The Dahlquist first barrier [1]).*

Theorem 3 *If k is even and the LM method with $(\alpha_j, \beta_j^{(0)})$ is of order $k+2$, then the FLM method (1) is also of order $k+2$.*

Proof If the assumption of this theorem is true then we have $C_{k+2}^{(0)} = 0$. Therefore the condition that the coefficient of h^{k+2} in (21) is being 0 means

$$\sum_{q=1}^{k+2} C_q^{(k+2-q)} \varphi_m^{(q-1)}(t) = \sum_{q=1}^{k+1} C_q^{(k+2-q)} \varphi_m^{(q-1)}(t) = 0, \quad m = 1, 2, \dots, k+1,$$

or equivalently

$$W^T \begin{pmatrix} C_1^{(k+1)} \\ C_2^{(k)} \\ \vdots \\ C_{k+1}^{(1)} \end{pmatrix} = 0, \quad (25)$$

which leads to

$$C_1^{(k+1)} = C_2^{(k)} = \dots = C_{k+1}^{(1)} = 0.$$

From this result together with $K = 0$, which has already been proved in Theorem 2, we have $C_q^{(l)} = 0$ for $1 \leq q+l \leq k+2$, which means that all the coefficients of h^j ($j = 0, 1, \dots, k+2$) in (21) are being 0. Thus we have proved that the FLM method is being of order $k+2$. ■

3 Coefficients of FLM

Next we consider t - and x - dependences of β_j .

Theorem 4 *The coefficients β_j ($j = 0, 1, \dots, k$) are independent of t , if and only if the functions $\varphi(t) = (\varphi_1(t), \dots, \varphi_{k+1}(t))^T$ are the solution of the constant coefficient linear equation*

$$\varphi'(t) = A\varphi(t), \quad (26)$$

or equivalently $\Phi(t) = (\Phi_1(t), \dots, \Phi_{k+1}(t))^T$ is the solution of the equation

$$\Phi'(t) = A\Phi(t) + b. \quad (27)$$

Proof (Sufficiency) Differentiating both sides of (6) with respect to t , we have

$$\rho(\Delta) \Phi'(t) = h \left(\frac{\partial \sigma}{\partial t} \Phi'(t) + \sigma(\Delta) \Phi''(t) \right).$$

On the other hand, (27) leads to

$$\begin{aligned} \rho(\Delta) \Phi'(t) &= \rho(\Delta) (A\Phi(t) + b) \\ &= \rho(\Delta) A\Phi(t) \\ &= h \sigma(\Delta) A\Phi'(t) \\ &= h \sigma(\Delta) \Phi''(t), \end{aligned}$$

where we use $\rho(1) = 0$. Comparing these two expressions, we have

$$\sum_{j=0}^k \frac{\partial \beta_j}{\partial t} \varphi_m(t + jh) = 0, \quad m = 1, 2, \dots, k+1,$$

which means that

$$C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1}) \begin{pmatrix} \frac{\partial \beta_0}{\partial t} \\ \frac{\partial \beta_1}{\partial t} \\ \vdots \\ \frac{\partial \beta_k}{\partial t} \end{pmatrix} = 0, \quad (28)$$

where $C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1})$ is the Casoratian matrix. Since C is nonsingular we have

$$\frac{\partial \beta_j}{\partial t} = 0, \quad j = 0, 1, \dots, k.$$

(Necessity) Let β_j be independent of t . Then the equation

$$C_{k+2}^{(0)} \varphi_m^{(k+1)}(t) + C_{k+1}^{(1)} \varphi_m^{(k)}(t) + \dots + C_1^{(k+1)} \varphi_m(t) = 0, \quad (29)$$

which is the condition that the coefficient of h^{k+2} in (21) is being 0, is the constant coefficient $(k+1)$ th order ordinary differential for $\varphi_m(t)$. Therefore $\varphi(t) = (\varphi_1(t), \varphi_2(t), \dots, \varphi_{k+1}(t))^T$

is the solution of the equation of the type (26) with the coefficient matrix A whose eigenvalues are given by the solutions of the algebraic equation

$$C_{k+2}^{(0)} \xi^{k+1} + C_{k+1}^{(1)} \xi^k + \cdots + C_1^{(k+1)} = 0. \quad (30)$$

■

Theorem 5 *The coefficients β_j are independent of h , if and only if $\varphi_m(t)$ ($m = 1, 2, \dots, k+1$) are linearly independent polynomials of degree $\leq k$.*

Proof (Sufficiency) First of all we consider the case that $\varphi_m(t) = t^{m-1}$, that is $\Phi_m(t) = m^{-1} t^m$ ($m = 1, 2, \dots, k+1$). Then $C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1})$ is a kind of Vandermonde matrix and is nonsingular for $h > 0$, and therefore β_j are uniquely determined. In this case $O(h^{k+1})$ and higher terms in (10) and (14) vanish, so that $\beta_j = \frac{\det C_j}{\det C}$ are independent of h .

Next we consider the general case that $\varphi_m(t)$ are the polynomials of degree $\leq k$ such that $C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1})$ is nonsingular for $t \in [t_0, T]$. Then if

$$\varphi_m(t) = \sum_{i=1}^{k+1} \gamma_{m,i} t^{i-1}, \quad m = 1, 2, \dots, k+1,$$

we obtain

$$C(t; \varphi_1, \varphi_2, \dots, \varphi_{k+1}) = \Gamma C(t; 1, t, \dots, t^k),$$

where

$$\Gamma = \begin{pmatrix} \gamma_{1,1} & \gamma_{1,2} & \cdots & \gamma_{1,k+1} \\ \gamma_{2,1} & \gamma_{2,2} & \cdots & \gamma_{2,k+1} \\ \cdots & \cdots & \cdots & \cdots \\ \gamma_{k+1,1} & \gamma_{k+1,2} & \cdots & \gamma_{k+1,k+1} \end{pmatrix}$$

Note that the non-singularity of $C(t; 1, t, \dots, t^k)$ means the non-singularity of Γ . Then the defining equation (4) of β_j is

$$\Gamma C(t; 1, t, \dots, t^k) \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} = h^{-1} \rho(\Delta) \begin{pmatrix} \Phi_1(t) \\ \Phi_2(t) \\ \vdots \\ \Phi_{k+1}(t) \end{pmatrix},$$

so that we have

$$C(t; 1, t, \dots, t^k) \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} = h^{-1} \rho(\Delta) \Gamma^{-1} \begin{pmatrix} \Phi_1(t) \\ \Phi_2(t) \\ \vdots \\ \Phi_{k+1}(t) \end{pmatrix} = h^{-1} \rho(\Delta) \begin{pmatrix} 1 \\ t \\ \vdots \\ t^{k+1} \end{pmatrix}. \quad (31)$$

This shows that β_j are the same as those obtained by t^{m-1} ($m = 1, 2, \dots, k+1$). Therefore the β_j generated by $\varphi_m(t)$ ($m = 1, 2, \dots, k+1$) are independent of h .

(Necessity) Next we assume β_j ($j = 0, 1, \dots, k$) are independent of h , that is $\beta_j = \beta_j^{(0)}$. Then we have $C_q = C_q^{(0)}$, and $\beta_j = \beta_j^{(0)}$ are determined uniquely by

$$C_q^{(0)} = \frac{1}{q!} \left(\sum_{j=0}^k \alpha_j j^q - q \sum_{j=0}^k \beta_j^{(0)} j^{q-1} \right) = 0, \quad q = 1, 2, \dots, k+1. \quad (32)$$

It is clear from the expression that the $\beta_j = \beta_j^{(0)}$ are also independent of t . Therefore from Theorem 4 we have that the generating functions $\varphi_m(t)$ are the solutions of some linear equation $\varphi'(t) = A\varphi(t)$. The linearly independent solutions (fundamental system) of the equation are given by

$$\varphi_{l,i}(t) = t^{i-1} \exp(\lambda_l t), \quad i = 1, \dots, m_l, \quad l = 1, \dots, r,$$

where λ_l is the eigenvalues of A with multiplicity m_l . Let assume that one of the eigenvalues, say λ , is nonzero, then one of the generating functions corresponding to λ is $\varphi_m(t) = \exp(\lambda t)$. Substituting this into (4) we have

$$\exp(\lambda t) \left(\sum_{j=0}^k \alpha_j \right) + \exp(\lambda t) \sum_{q \geq 1} \frac{(\lambda h)^q}{q!} \left(\sum_{j=0}^k \alpha_j j^q - q \sum_{j=0}^k \beta_j^{(0)} j^{q-1} \right) = 0.$$

This means that (32) holds even for $q > k+1$, which violates the order barrier. Thus all the eigenvalues of A are 0, i.e. $\varphi_m(t)$ are polynomials of degree $\leq k$. ■

4 Adams type FLM method

In this section we consider Adams type FLM method. Let the first characteristic polynomial $\rho(\zeta)$ be

$$\rho(\zeta) = \zeta^k - \zeta^{k-1}.$$

In this case the order of the FLM method is $k+1$, whatever the parity of k .

Consider the linear equation

$$y'' = -y + \varepsilon \cos t, \quad y(0) = 1, \quad y'(0) = 0. \quad (33)$$

The exact solution of the equation is given by

$$y(t) = \cos t + \frac{1}{2} \varepsilon t \sin t.$$

Here we solve the equation with $\varepsilon = 0.5$ by the two methods, 1- and 2-step Adams type FLM methods. In this case we use the PECE mode in which the predictors are explicit Adams type and the correctors are implicit Adams type. The global errors of these two methods are shown in Figures 1 and 2.

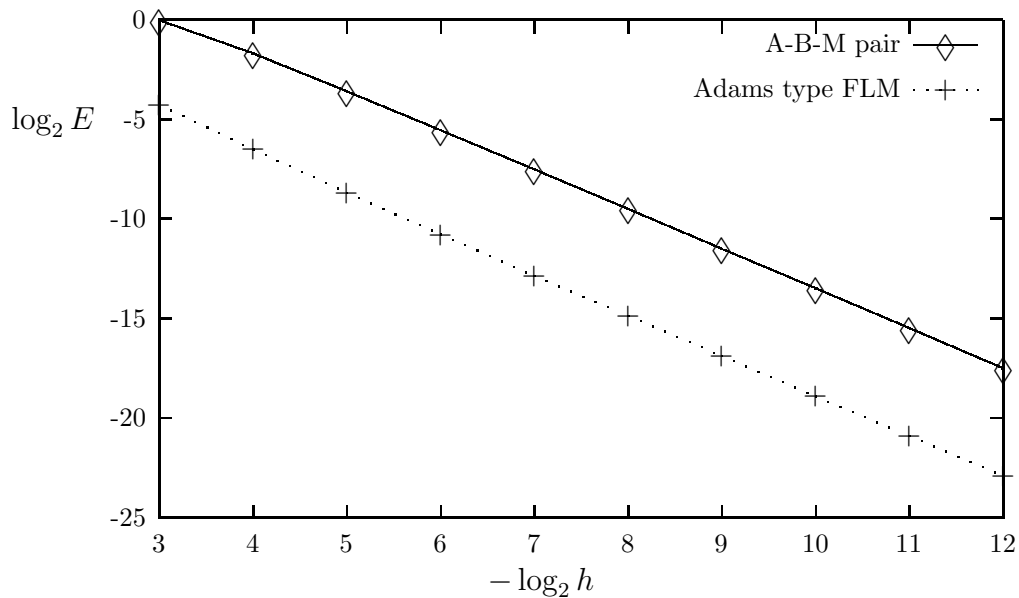


Figure 1 Global errors of PECE Adams type FLM method of order 2.

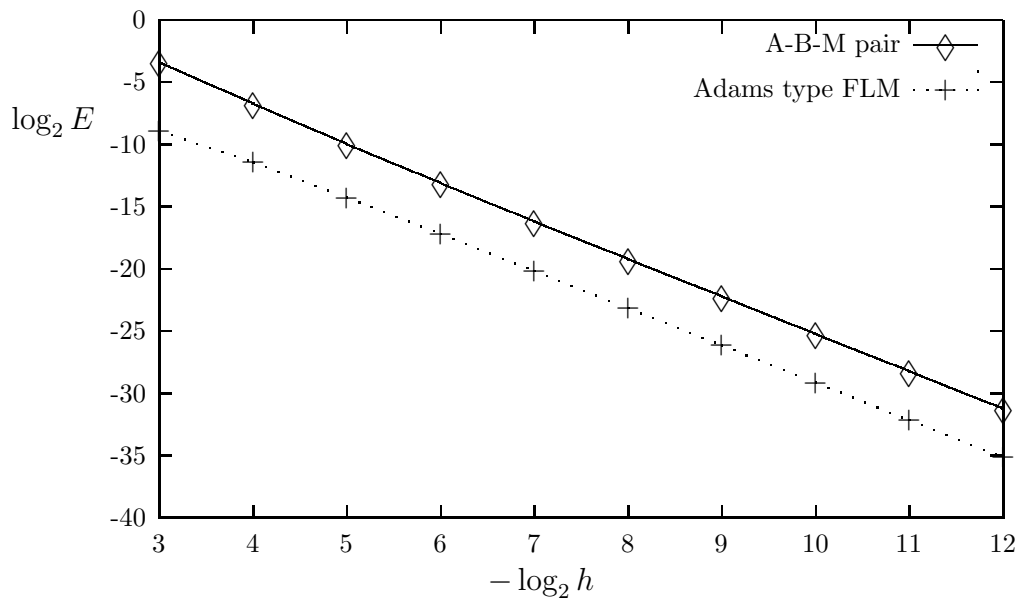


Figure 2 Global errors of PECE Adams type FLM method of order 3.

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