A Class of Lobatto Methods of Order 2*s*

Wang Fangzong and Liao Xiaobing

***Abstract*—The families of Lobatto Runge-Kutta methods that consist of Lobatto IIIA methods, Lobatto IIIB methods, and Lobatto IIIC methods are all of order 2*s*−2 and A-stable. Using *V*- transformation and the method of undetermined coefficients, a class of Lobatto Runge-Kutta methods of order 2*s* and A-stable are constructed through converting its stability function into diagonal Padé approximation to *exp*(*z*). The two numerical examples also show that the derived new Lobatto methods have higher accuracy than traditional Lobatto methods.**

***Index Terms*—Lobatto methods, order, *V*-transformation, Padé approximation**

I. Introduction

Lobatto Runge-Kutta methods [1]-[4] for the numerical integration of ordinary differential equations are named after Rehuel Lobatto. They are characterized by the use of approximations to the solution at the two end points t_n and t_{n+1} of each subinterval of integration $[t_n, t_{n+1}]$. One of well-known Lobatto methods is the implicit trapezoidal rule, which has been widely used in practice.

Consider a system of ordinary differential equations (ODEs)

$$\begin{cases} \dfrac{dx}{dt} = f(t,x),\ 0 < t \le T \\ x(t=0) = x_0 \end{cases} \tag{1}$$

Starting from x_0 at t_0 one step $(t_n, x_n) \to (t_{n+1}, x_{n+1})$ of the *s*-stage Lobatto Runge-Kutta methods applied to (1) can be expressed as follows

$$\tilde{x}_i = x_n + h\sum_{j=1}^{s} a_{ij} f(t_n + c_j h, \tilde{x}_j), i \in (1,s) \tag{2}$$

$$x_{n+1} = x_n + h\sum_{j=1}^{s} b_j f(t_n + c_j h, \tilde{x}_j) \tag{3}$$

where the stage value s satisfies $s \ge 2$ and the coefficients a_{ij}, b_j, c_j characterize the Lobatto Runge-Kutta methods. The s intermediate values $\tilde{x}_i, i \in (1,s)$ are called the internal stages and can be considered as approximations to the solution at $t_n + c_i h$. Lobatto Runge-Kutta methods are characterized by $c_1 = 0$ and $c_s = 1$.

The families of traditional Lobatto methods involve Lobatto IIIA methods, Lobatto IIIB methods, and Lobatto IIIC methods. A comprehensive review about Lobatto methods can be found in Reference [1]-[3] and can be summarized in Table 1.

TABLE I
A Summary Of Traditional Lobatto Methods

methods	simplifying assumptions	order	stability functions
Lobatto IIIA	B(2*s*−2), C(*s*), D(*s*−2)	2*s*−2	(*s*−1, *s*−1)−Padé
Lobatto IIIB	B(2*s*−2), C(*s*−2), D(*s*)	2*s*−2	(*s*−1, *s*−1)−Padé
Lobatto IIIC	B(2*s*−2), C(*s*−1), D(*s*−1)	2*s*−2	(*s*−2, *s*)−Padé

However, these traditional Lobatto methods are all of order 2*s*−2 and A-stable; they have the disadvantages of lower calculation precision when comparing with Gauss methods of order 2*s*. In this paper, we devoted to construct a class of new Runge-Kutta methods based on Lobatto quadrature formulas [5] whose order can be highest of 2*s*.

II. Lobatto Quadrature Formulas

For a given number of stages *s*, the various Lobatto methods have the same coefficients ***b*** and ***c*** based on the corresponding Lobatto quadrature formula [6]. The solution of (1) can be approximated by using a standard quadrature formula:

$$\begin{aligned} x_{n+1} &= x_n + \int_{t_n}^{t_{n+1}} f(t, x(t))\,dt \\ &= x_n + h\left(\sum_{i=1}^{s} b_i f(t_n + c_i h, x(t_n + c_i h))\right) \end{aligned} \tag{4}$$

with *s* node coefficients $c_1, c_2, \ldots c_s$, and *s* weight coefficients $b_1, b_2, \ldots b_s$. Lobatto quadrature formulas, also known as Gauss-Lobatto quadrature formulas in the literature, are given for $s \ge 2$ by a set of nodes and weights satisfying conditions described hereafter. The s nodes c_i are the roots of the polynomial of degree *s*

$$\frac{d^{s-2}}{dt^{s-2}}(t^{s-1}(1-t)^{s-1}) \tag{5}$$

Those nodes satisfy $c_1 = 0 < c_2 < \ldots < c_s = 1$. The weights

Manuscript received June 12, 2015; revised August 25, 2015. This work was supported by the National Natural Science Foundation of China under Grant No. 51377098 and 50977052.

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b_i and nodes c_i satisfy the condition B (2s−2) where

$$B(p):\ \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k},\ \text{for } k = 1, 2, \ldots, p \tag{6}$$

Lobatto quadrature formulas are symmetric, i.e., their nodes and weights satisfy

$$b_{s+1-j} = b_j,\ c_{s+1-j} = 1 - c_j,\ \text{for } j = 1, 2, \ldots, s \tag{7}$$

The families of Lobatto Runge-Kutta methods described above differ only in the values of their coefficients matrix $\boldsymbol{A}$. The coefficients matrix $\boldsymbol{A}$ of these families can be linearly implicitly defined with the help of so-called simplifying assumptions [3]

$$C(q):\ \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k},\ \text{for } i = 1, 2, \ldots, s \text{ and } k = 1, 2, \ldots, q \tag{8}$$

$$D(r):\ \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j}{k}(1 - c_j^k),\ \text{for } j = 1, 2, \ldots, s \text{ and } k = 1, 2, \ldots, r \tag{9}$$

The importance of these simplifying assumptions comes from a fundamental result due to Butcher. The coefficients a_{ij}, b_j, c_j characterizing the Lobatto Runge-Kutta methods (2)-(3) can be arranged into the form of a table called a Butcher tableau [3]

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \tag{10}$$

III. Construction Of A Class Of Lobatto Methods Of Order 2s

As is well-known that, if the stability function of an s-stage Runge-Kutta method is (s,s)-Padé approximation to $exp(z)$ [7], then this method is of order 2s and A-stable. Inspired by this, the stability functions of new Lobatto methods are converted into diagonal Padé approximation to $exp(z)$ by using the method of undetermined coefficients, so naturally, this class of new Lobatto methods are of order 2s and A-stable.

Without changing the coefficients $\boldsymbol{b}$ and $\boldsymbol{c}$, an s-stage new Lobatto method is defined as

$$\begin{array}{c|c} \boldsymbol{c} & \tilde{\boldsymbol{A}} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} = \begin{array}{c|c} \boldsymbol{c} & \boldsymbol{V}_s \tilde{\boldsymbol{A}}_s \boldsymbol{V}_s^{-1} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} \tag{11}$$

where

$$\boldsymbol{V}_s = \begin{pmatrix} 1 & c_1 & \cdots & c_1^{s-1} \\ 1 & c_2 & \cdots & c_2^{s-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & c_s & \cdots & c_s^{s-1} \end{pmatrix} \tag{12}$$

$$\tilde{\boldsymbol{A}}_s = \begin{pmatrix} 0 & 0 & 0 & \cdots & \tilde{\alpha}_1 \\ 1 & 0 & 0 & \cdots & \tilde{\alpha}_2 \\ 0 & \frac{1}{2} & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & \frac{1}{s-1} & \tilde{\alpha}_s \end{pmatrix} \tag{13}$$

Equation $\tilde{\boldsymbol{A}} = \boldsymbol{V}_s \tilde{\boldsymbol{A}}_s \boldsymbol{V}_s^{-1}$ is the famous "$\boldsymbol{V}$-transformation" [8], [9]. Suppose that new Lobatto method satisfies symmetry condition $\boldsymbol{PAP} = \boldsymbol{eb}^{\mathrm{T}} - \boldsymbol{A}$ [10], then, the stability function of new Lobatto method can be calculated by

$$\begin{aligned} R(z) &= \frac{\det(\boldsymbol{I} + z(\boldsymbol{eb}^{\mathrm{T}} - \tilde{\boldsymbol{A}}))}{\det(\boldsymbol{I} - z\tilde{\boldsymbol{A}})} = \frac{\det(\boldsymbol{I} + z(\boldsymbol{P}\tilde{\boldsymbol{A}}\boldsymbol{P}))}{\det(\boldsymbol{I} - z\tilde{\boldsymbol{A}})} \\ &= \frac{\det(\boldsymbol{I} + z\tilde{\boldsymbol{A}})}{\det(\boldsymbol{I} - z\tilde{\boldsymbol{A}})} = \frac{\det(\boldsymbol{I} + z\tilde{\boldsymbol{A}}_s)}{\det(\boldsymbol{I} - z\tilde{\boldsymbol{A}}_s)} \end{aligned} \tag{14}$$

Due to $\tilde{\boldsymbol{A}}_s$ being a matrix with special structure, (14) can be further expressed as

$$R(z) = \frac{1 - \sum_{k=s}^{1} \tilde{\alpha}_k \frac{(k-1)!}{(s-1)!}(-z)^{s-k+1}}{1 - \sum_{k=s}^{1} \tilde{\alpha}_k \frac{(k-1)!}{(s-1)!} z^{s-k+1}} \tag{15}$$

Let $R(z)$ equal to (s,s)-Padé approximation to $exp(z)$ denoted by e_s^z, i.e.

$$\frac{1 - \sum_{k=s}^{1} \tilde{\alpha}_k \frac{(k-1)!}{(s-1)!}(-z)^{s-k+1}}{1 - \sum_{k=s}^{1} \tilde{\alpha}_k \frac{(k-1)!}{(s-1)!} z^{s-k+1}} = e_s^z \tag{16}$$

Comparing the corresponding polynomial coefficients on both sides of (16), it can be inferred that

$$\begin{pmatrix} 1 & \frac{1}{2} & \cdots & \frac{1}{s} \\ \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{s+1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{s} & \frac{1}{s+1} & \cdots & \frac{1}{2s-1} \end{pmatrix} \begin{pmatrix} \tilde{\alpha}_1 \\ \tilde{\alpha}_2 \\ \vdots \\ \tilde{\alpha}_s \end{pmatrix} = \begin{pmatrix} \frac{1}{s(s+1)} \\ \frac{1}{s(s+2)} \\ \vdots \\ \frac{1}{s(s+s)} \end{pmatrix} \tag{17}$$

Obviously, (17) can be further simplified to

$$\sum_{j=1}^{s} \frac{\tilde{\alpha}_j}{k+j-1} = \frac{1}{s(s+k)},\ \text{for } k = 1, 2 \ldots, s \tag{18}$$

Therefore, when the coefficients $\tilde{\boldsymbol{\alpha}}_s = (\tilde{\alpha}_1, \tilde{\alpha}_2, \ldots, \tilde{\alpha}_s)$ of new Lobatto method satisfy (18), then its stability function is (s,s)-Padé approximation to $exp(z)$, so naturally, this Lobatto method is the method of order 2s.

Gauss method is a good example for the proposed construction method. *S-stage* Gauss method satisfies (18) and its stability function is (s,s)-Padé approximation to $exp(z)$. Equation (18) has an unique solution for a given s, for example $s = 2 \sim 4$, $\tilde{\boldsymbol{\alpha}}_s$ are given by

$$s=2,\ \tilde{\boldsymbol{\alpha}}_2 = (-1/12, 1/2),$$

$$s=3,\ \tilde{\boldsymbol{\alpha}}_3 = (1/60, -1/5, 1/2),$$

$$s=4,\ \tilde{\boldsymbol{\alpha}}_4 = (-1/280, 1/14, -9/28, 1/2),$$

……

Now, s-stage $2s$-order Lobatto methods with s = 2, 3, 4 are listed below

$$s=2,\ \begin{array}{c|c} \boldsymbol{c} & \tilde{\boldsymbol{A}} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} = \begin{array}{c|cc} 0 & \frac{1}{12} & -\frac{1}{12} \\ 1 & \frac{7}{12} & \frac{5}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$$s=3,\ \begin{array}{c|c} \boldsymbol{c} & \tilde{\boldsymbol{A}} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} = \begin{array}{c|ccc} 0 & \frac{1}{30} & -\frac{1}{15} & \frac{1}{30} \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{2}{15} & \frac{11}{15} & \frac{2}{15} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

$$s=4,\ \begin{array}{c|c} \boldsymbol{c} & \tilde{\boldsymbol{A}} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array} = \begin{array}{c|cccc} 0 & \frac{1}{56} & -\frac{\sqrt{5}}{56} & \frac{\sqrt{5}}{56} & -\frac{1}{56} \\ \frac{5-\sqrt{5}}{10} & \frac{37}{420}+\frac{\sqrt{5}}{120} & \frac{5}{24}-\frac{\sqrt{5}}{210} & \frac{5}{24}-\frac{47\sqrt{5}}{420} & -\frac{1}{210}+\frac{\sqrt{5}}{120} \\ \frac{5+\sqrt{5}}{10} & \frac{37}{420}-\frac{\sqrt{5}}{120} & \frac{5}{24}+\frac{47\sqrt{5}}{420} & \frac{5}{24}+\frac{\sqrt{5}}{210} & -\frac{1}{210}-\frac{\sqrt{5}}{120} \\ 1 & \frac{17}{168} & \frac{5}{12}-\frac{\sqrt{5}}{56} & \frac{5}{12}+\frac{\sqrt{5}}{56} & \frac{11}{168} \\ \hline & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{array}$$

To the author’s knowledge about Runge-Kutta methods, the Lobatto methods of order $2s$ and A-stable described above have so far not been reported. So, for convenience this class of Lobatto methods are named hereafter Lobatto IIIF methods.

What’ more, the construction method based on $\boldsymbol{V}$-transformation and described above can similarly be applied to construction of $2s$–order Radau methods. Interestingly, when the construction method adopts coefficients $\boldsymbol{c}$ and $\boldsymbol{b}$ of traditional Radau IA methods, new Runge-Kutta methods are Radau IB methods [11], [12], when the construction method adopts coefficients $\boldsymbol{c}$ and $\boldsymbol{b}$ of traditional Radau IIA methods, new Runge-Kutta method are Radau IIB methods[11], [12]. Radau IB methods and Radau IIB methods were first proposed by Sun Geng [11], [12] using $\boldsymbol{W}$-transformation [2]. However, their stability functions are changed into (s,s)-Padé approximation to $exp(z)$, instead of $(s-1,s)$-Padé approximation. Therefore, Radau IB methods and Radau IIB methods are not the method of order $2s-1$ but order $2s$.

IV. Numerical Experiments

In this section, we give two simple examples to illustrate our main results obtained in previous sections.

Example 1. Consider a two-degree-of-freedom system governed by

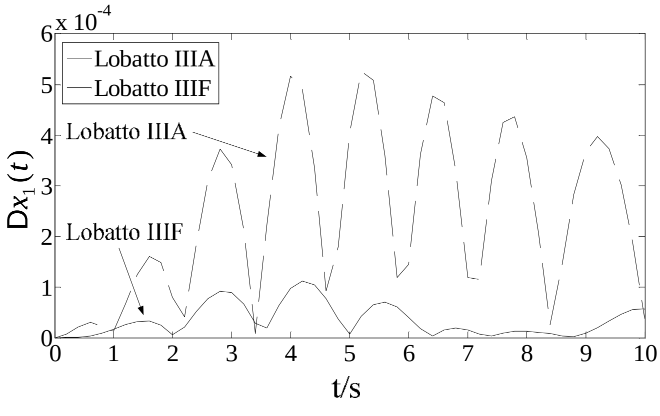
$$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{Bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{Bmatrix} + \begin{pmatrix} 6 & -2 \\ -2 & 4 \end{pmatrix}\begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 5\cos(3t) \end{Bmatrix} \tag{19}$$

with initial condition $x_1(0) = x_2(0) = 0$, $\dot{x}_1(0) = \dot{x}_2(0) = 0$

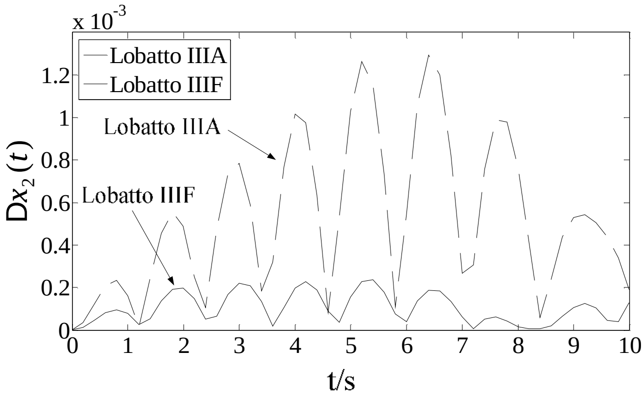
and the exact solution of the problem is

$$\begin{cases} x_1 = \frac{5}{28}\cos(3t) + \frac{5}{21}\cos(\sqrt{2}t) - \frac{5}{12}\cos(\sqrt{5}t) \\ x_2 = -\frac{15}{14}\cos(3t) + \frac{5}{21}\cos(\sqrt{2}t) + \frac{5}{6}\cos(\sqrt{5}t) \end{cases} \tag{20}$$

With the exact solution (20) as a reference, error trajectories will be observed and tracked using four kinds of Lobatto methods (error denoted by $\Delta x_1(t)$ and $\Delta x_2(t)$). Fig.1 shows the displacement error trajectories comparison of Lobatto IIIA method and Lobatto IIIF method. Fig.2 shows the displacement error trajectories comparison of Lobatto IIIB method and Lobatto IIIF method. Fig.3 shows the displacement error trajectories comparison of Lobatto IIIC method and Lobatto IIIF method. From Figs.1-3, it has been shown that Lobatto IIIF method has higher calculation accuracy than all the traditional Lobatto methods.

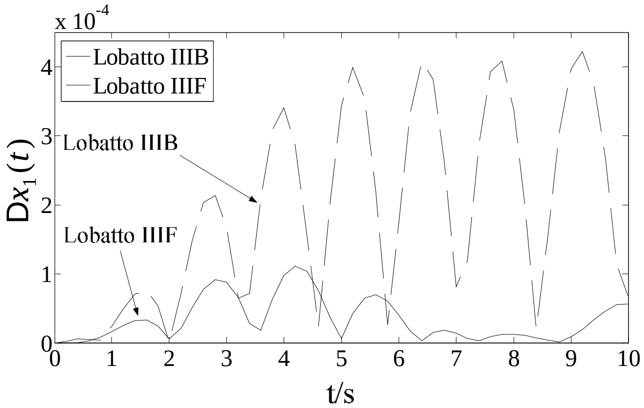


(a) Error trajectories of $x_1(t)$

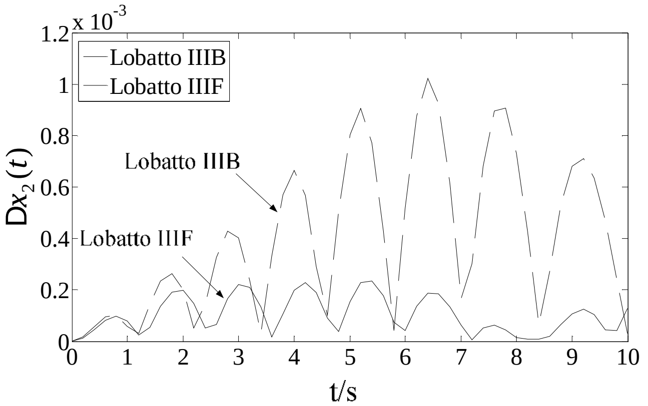


(b) Error trajectories of $x_2(t)$

Fig. 1 Error trajectories comparison of Lobatto IIIA method and Lobatto IIIF method (s=3, h=0.2s)

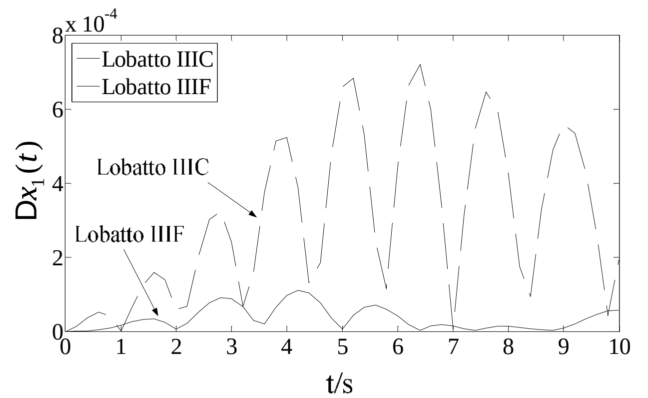


(a) Error trajectories of $x_1(t)$

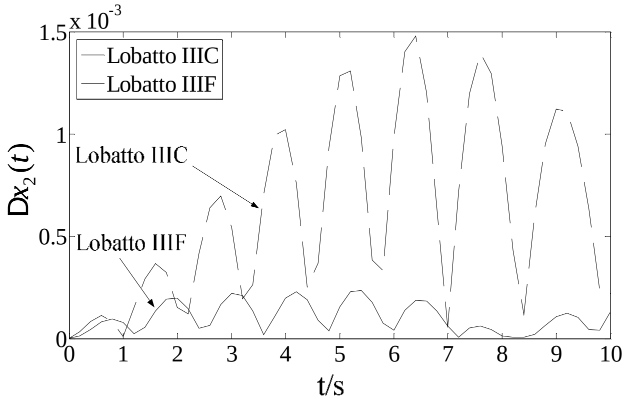


(b) Error trajectories of $x_2(t)$

Fig. 2 Error trajectories comparison of Lobatto IIIB method and Lobatto IIIF method (s=3, h=0.2s)



(a) Error trajectories of $x_1(t)$



(b) Error trajectories of $x_2(t)$

Fig. 3 Error trajectories comparison of Lobatto IIIC method and Lobatto IIIF method (s=3, h=0.2s)

Example 2. Consider a hardening elastic spring. The nonlinear dynamic equation is

$$\ddot{x} + s_1 x(1 + s_2 x^2) = 0 \tag{21}$$

where $s_1 > 0$, $s_2 > 0$. The exact total energy is

$$E = (2\dot{x}^2 + 2s_1 x^2 + s_1 s_2 x^4)/4 \tag{22}$$

To assess the time integration numerical methods, the percent error in terms of the energy was introduced [12],

$$E_r = \left|(E - E_0)/E_0\right| \times 100\% \tag{23}$$

where E_0 is the total energy at $t = 0$. For numerical results present herein, $s_1 = 100$, $s_2 = 10$. The initial conditions are $\dot{x}_0 = 1.5$ and $x_0 = 0$.

Table 2 lists the maximum percentage errors of the total energy over the time duration of 20s. The results of four kinds of Lobatto methods are obtained with s=3 and the Newton method that is used in solving the nonlinear algebraic equations.

TABLE II
MAXIMUM PERCENTAGE ERRORS OF THE TOTAL ENERGY DURING 20S

step size h	0.2s	0.1s	0.05s	0.01s
Lobatto IIIF	26.9	5.6	0.0	0.0
Lobatto IIIA	33.8	6.8	0.3	0.0
Lobatto IIIB	35.3	7.0	0.2	0.0
Lobatto IIIC	34.6	7.3	0.4	0.0

It can be also seen from Table 2 that the Lobatto IIIF method has higher calculation accuracy than all the traditional Lobatto methods. Accurate results can be obtained with much larger step size using Lobatto methods.

V. CONCLUSION

A class of Lobatto methods of order 2s and A-stable have been successfully constructed and numerical examples have shown that new Lobatto methods are more precise than traditional Lobatto methods of order 2*s*–2. The construction method based on ***V***-transformation can be also applied to construction of 2*s*–order Radau methods. It has been found that 2*s*–order Radau methods are Radau IB methods and Radau IIB methods, whose stability functions are (*s*,*s*)–Padé approximation to *exp*(*z*).

ACKNOWLEDGMENT

The authors would like to thank the anonymous referees for their helpful comments and valuable suggestions, which led to the improvement of the manuscript.

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