Higher Order Symplectic Methods Based on the Modified Vector Fields

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The higher-order, structure-preserving numerical integrators based on the modified vector fields (backward error analysis) are used to construct discretizations of separable systems. This new approach is called as modifying integrators. As an example of modifying integrator Lobatto III-A and III-B are chosen. These new efficient higher-order numerical integrators are applied to the separable Hamiltonian equations.

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Key Words: structure-preserving numerical integrators, Lobatto III-A and III-B integrator, separable Hamiltonian equations.

1. Introduction

In recent years, geometric numerical integration methods have come\textsuperscript{[1]} to the fore, partly as an alternative to traditional methods such as Runge-Kutta methods. A numerical method is called geometric integrator if it preserves one or more physical/geometric properties of the system exactly (i.e up to roundoff error). Examples of such geometric properties\textsuperscript{[4]} that can be preserved are (first) integrals, symplectic structure, symmetries and reversing-symmetries, phase-space volume, Lyapunov functions, foliations, e.t.c.

In the literature symplectic methods are generally constructed using generating functions, Runge-Kutta methods, splitting methods and variational methods. One of the methods for constructing high-order symplectic integrators is developed by using the idea of backward error analysis while constructing modified equations by inverting the roles of the exact and numerical flows. The idea given in\textsuperscript{[1]} is presented as follows: We consider an initial value problem

\begin{equation}
\dot{y} = f(y), \quad y(0) = y_0
\end{equation}

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where $f \in C^\infty[\mathbb{R}^n]$ and a numerical one-step integrator $y_{n+1} = \Phi_{f,h}(y_n)$. We search for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + h f_2(z) + h^2 f_3(z) + \ldots, \quad z(0) = y_0$$  \hspace{1cm} (2)$$

such that the numerical solution $\{z_n\}$ of the method applied with step size $h$ to (2) yields formally the exact solution of the original differential equation (1), i.e. $z_n = y(nh)$ for $n = 0, 1, 2, \ldots$ The coefficient functions $f_j(z)$ can be computed recursively.

Having found first functions $f_j(z)$, one can use the truncation

$$\dot{z} = f_h^{[r]}(z) = f(z) + h f_2(z) + \ldots + h^{r-1} f_r(z)$$  \hspace{1cm} (3)$$
of the modified differential equation corresponding to $\Phi_{f,h}(y)$. A numerical method $z_{n+1} = \Phi_{f_h^{[r]},h}(z_n)$ approximates the solution of (1) with order $r$. It was called a modifying integrator because it applies to the modified vector field $f_h^{[r]}$ instead of $f(y)$. In this study we mainly consider the partitioned and separable systems given in (4) and (5),

$$\begin{cases}
y' = f(y, z) \\
z' = g(y, z)
\end{cases}$$  \hspace{1cm} (4)$$

$$\begin{cases}
y' = f(z) \\
z' = g(y)
\end{cases}$$  \hspace{1cm} (5)$$

In particular, we will be interested in canonical Hamiltonian equations, which are generated by a Hamiltonian function $H(y, z)$:

$$f(y, z) = H_z(y, z), \quad g(y, z) = -H_y(y, z)$$  \hspace{1cm} (6)$$

Such system often arise in mechanical systems described by a Hamiltonian function

$$H = \frac{p^2}{2} + V(q),$$

which provides us with the Hamiltonian equations of motion

$$\begin{cases}
x' = p \\
p' = -V_q(q)
\end{cases}$$  \hspace{1cm} (7)$$

In next section we construct the higher order method corresponding to Lobatto IIIA-IIIB method by using the modified vector fields.
2. Construct of Higher Order Modified Lobatto IIIA – IIIB pair

In this section we will construct higher order method corresponding to Lobatto IIIA-IIIB pair of method. Our Lobatto IIIA - IIIB pair of order 2 is given as follows:

\[ k_1 = f \left( y_0, z_0 + \frac{h}{2} l_1 \right), \quad k_2 = f \left( y_0 + \frac{h}{2} (k_1 + k_2), z_0 + \frac{h}{2} l_1 \right), \]

\[ l_1 = g \left( y_0, z_0 + \frac{h}{2} l_1 \right), \quad l_2 = g \left( y_0 + \frac{h}{2} (k_1 + k_2), z_0 + \frac{h}{2} l_1 \right), \]

\[ y_1 = y_0 + \frac{h}{2} (k_1 + k_2), \quad z_1 = z_0 + \frac{h}{2} (l_1 + l_2). \]

In the case of separable equations this method gets reduced to an explicit form known as Störmer–Verlet scheme.

The modified differential equations are

\[
\begin{align*}
\dot{y} &= f(y, z) + h^2 a(y, z), \\
\dot{z} &= g(y, z) + h^2 b(y, z),
\end{align*}
\]

where

\[ a(y, z) = \frac{1}{12} \left( -f_{yy}(f, f) + f_{yz}(f, g) + \frac{1}{2} f_{zz}(g, g) - f_y f_y f - f_y f_z g + 2 f_z g_y f - f z g g \right) \]

\[ b(y, z) = \frac{1}{12} \left( -g_{yy}(f, f) + g_{yz}(f, g) + \frac{1}{2} g_{zz}(g, g) - g_y f f - g_y f z g + 2 g_z g_y f - g z g g \right) \]

If the original equations are Hamiltonian, then the modified differential equations (8) are generated by the Hamiltonian function

\[ H^{[3]} = H + \frac{h^2}{12} \left( -H_{yy}(f, f) + H_{yz}(f, g) + \frac{1}{2} H_{zz}(g, g) \right), \]

where \( f \) and \( g \) are given by (6).

The modified differential equations for separable systems are simplified:
If the original equations are Hamiltonian, the modified differential equations are generated by

\[ H^{[3]} = H + \frac{h^2}{12} \left( -H_{yy}(f, f) + \frac{1}{2}H_{zz}(g, g) \right) \]

For mechanical system, equation (7) can be

\[ H^{[3]} = H + \frac{h^2}{12} \left( -V_{qq}(p, p) + \frac{1}{2}(V_q, V_q) \right) \]

The modified equations take the form

\[
\begin{cases}
q' = p + \frac{h^2}{6} g_q p = \left( I - \frac{h^2}{6} V_{qq} \right) p \\
p' = -V_q(q) - \frac{h^2}{12} (g_{qq}(p, p) + g_q g) 
\end{cases}
\]

Application of Lobatto IIIA - IIIB pair of order 2 to these equations leads to a scheme which can be split into three stages:

\[ p_{1/2} = p_0 + \frac{h}{2} \left( g(q_0) - \frac{h^2}{12} \left( g_{qq}(q_0)(p_{1/2}, p_{1/2}) + g_q(q_0)g(q_0) \right) \right), \]

\[ q_1 = q_0 + h \left( I + \frac{h^2}{12} (g(q_0) + g(q_1)) \right) p_{1/2}, \]

\[ p_1 = p_{1/2} + \frac{h}{2} \left( g(q_1) - \frac{h^2}{12} \left( g_{qq}(q_1)(p_{1/2}, p_{1/2}) + g_q(q_1)g(q_1) \right) \right), \]

where we introduced an intermediate variable

\[ p_{1/2} = p_0 + \frac{h}{2} l_1. \]

Note that the first and second stages are implicit and the third is explicit.
3. Order of the Modified Lobatto Method


Proof. Consider the mechanical system as we mentioned before given in the equations (5),

\[ \dot{q} = p \]
\[ \dot{p} = -V_q(q) \]

Applying the Hamiltonian equation to mechanical system gives

\[
\begin{cases}
  q' = p + \frac{h^2}{6} g_p q = \left(I - \frac{h^2}{6} V_{qq}\right)p \\
  p' = -V_q(q) - \frac{h^2}{12} (g_{qq}(p,p) + g_{qg})
\end{cases}
\]

Since Lobatto IIIA - IIIB pair of order 2 is given as follows:

\[
k_1 = f(q_0, p_0 + \frac{h}{2} l_1) , \quad k_2 = f(q_0 + \frac{h}{2} (k_1 + k_2), p_0 + \frac{h}{2} l_1),
\]

\[
l_1 = g(q_0, p_0 + \frac{h}{2} l_1) , \quad l_2 = g(q_0 + \frac{h}{2} (k_1 + k_2), p_0 + \frac{h}{2} l_1),
\]

\[ q_{n+1} = q_n + \frac{h}{2} (k_1 + k_2), \quad p_{n+1} = p_n + \frac{h}{2} (l_1 + l_2). \]

The Taylor expansions of \( k_1, k_2, l_1, l_2 \) are:

\[
k_1 = f(q_0, p_0) + \frac{h}{2} l_1 \frac{\partial f}{\partial q}(q_0, p_0) + \frac{h^2}{2!} l_1^2 \frac{\partial^2 f}{\partial q^2}(q_0, p_0) + \ldots
\]

\[
= p_0 - \frac{h^2}{2} g_p p_0 + h l_1 - \frac{h^3}{6} l_1 g_q
\]

We need to find \( l_1 \), since we use \( l_1 \) in \( k_1 \):

\[
l_1 = -V_q(q_0) - \frac{h^2}{12} (g_{qq}(p_0, p_0) + g_{qg}) + \frac{h}{2} l_1 [-V_{qq}(q_0) - \frac{h^2}{12} (g_{qqq}(p_0, p_0) + g_{qqg} + g_{qg}^2)] + \ldots
\]

\[ q_1 = q_0 + \frac{h}{2} (k_1 + k_2) \] and since \( k_1 = k_2 \), then

\[
q_1 = q_0 + \frac{h}{2} (k_1 + k_2) = q_0 + h p_0 - \frac{h^3}{6} g_p p_0 + h^2 (-V_q(q_0) - \frac{h^2}{12} g_{qq}(p_0, p_0) - \frac{h^2}{12} g_q g + \ldots) -
\]
\[ -\frac{h^4}{6}(-V_q(q_0) - \frac{h^2}{12} g_{qq}(p_0, p_0) - \frac{h^2}{12} g_q g + \ldots) g_q \]

Our exact solution of \( \dot{q} = p + \frac{h^2}{6} g_q p \) is

\[ q(t_0 + h) = q(t_0) + h\dot{q}(t_0) + \frac{h^2}{2!} \ddot{q}(t_0) + \frac{h^3}{3!} q^{(3)}(t_0) + \frac{h^4}{4!} q^{(4)}(t_0) + \ldots \]

Substituting \( \dot{q} = p + \frac{h^2}{6} g_q p \) in taylor series expansion, we get

\[ q(t_0 + h) = q_0 + h(p_0 - \frac{h^2}{6} g_q p_0) + \frac{h^2}{2!} (-V_q(q_0) - \frac{h^2}{6} g_q g - \frac{h^2}{6} g_q g) \]

\[ + \frac{h^3}{3!} (-\frac{h^2}{6} g_{qq q} - \ldots) + \frac{h^4}{4!} (V_q(q_0) + \frac{h^2}{3} g_q g_q + \frac{h^2}{3} g_q^2) + \ldots \]

Subtracting \( q_1 \) from \( q(t_0 + h) \), we get \( \frac{h^3}{3!} (-\frac{h^2}{6} g_{qq q} - \ldots) = C_1 h^5 \) completes first part of proof.

For the second part of proof, we need \( l_1 \).

\[ l_1 = g(q_0, p_0 + \frac{h}{2} l_1) = g(q_0, p_0) + \frac{h}{2} l_1 g_q + \frac{h^2}{4} l_1^2 g_q + \ldots \]

\[ l_1 = -V_q(q_0) - \frac{h^2}{12} g_{qq}(p_0, p_0) + \frac{h}{2} l_1 [V_q(q_0) - \frac{h^2}{12} (g_{qq q}(p_0, p_0) + g_q g + g_q^2)] + \ldots \]

\[ \downarrow \]

\[ l_1 = -V_q(q_0) - \frac{h^2}{12} g_{qq}(p_0, p_0) - \frac{h^2}{12} g_q g - \frac{h^2}{2} g V_q(q_0) - \frac{h^3}{24} g_{qq q} g - \frac{h^3}{24} g_q g_q^2 - \]

\[ - \frac{h^3}{24} g_q^2 g + \frac{h^2}{4} g_q g_q + \ldots \]

and

\[ l_2 = g(q_0 + \frac{h}{2} (k_1 + k_2), p_0 + \frac{h}{2} l_1) = \]

\[ = -V_q(q_0 + h p_0 - \frac{h^3}{6} g_q p_0 + h^2 g - \frac{h^4}{6} g_q g) - h^2 \frac{12}{12} (g_{qq}(p_0, p_0) + g_q g) + \frac{h}{2} g_q g + \frac{h^2}{4} g_q g_q + \ldots \]

Since

\[ p_1 = p_0 + \frac{h}{2} (l_1 + l_2) = \]

\[ = p_0 - h V_q(q_0) - \frac{h^3}{12} g_{qq}(p_0, p_0) - \frac{h^3}{12} g_q g - \frac{h^2}{2} V_q(q_0) - \frac{h^4}{24} g_{qq q}(p_0, p_0) - \]

\[ - \frac{h^4}{24} g_q g_q - \frac{h^4}{24} g_q^2 - \frac{h^3}{6} V_{qq q} + \ldots \]
Our exact solution of \( \dot{p} = -V_q(q) - \frac{h^2}{12} (g_{qq}(p,p) + g_{qq}g) \) is

\[
p(t_0 + h) = p_0 + h(-V_q(q_0) - \frac{h^2}{12} g_{qq}(p_0,p_0) - \frac{h^2}{12} g_{qq}g) + \frac{h^2}{2!}(-V_{qq}(q_0) - \frac{h^2}{12} g_{qqq}(p_0,p_0) - \frac{h^2}{12} g_{qq}g - \frac{h^2}{12} g_{qq}g) + \frac{h^3}{3!}(-V_{qqq}(q_0,q_0) - \frac{h^2}{12} g_{qqqq}(p_0,p_0) - \frac{h^2}{12} g_{qqq}g - \frac{h^2}{12} g_{qq}g - \cdots) + \frac{h^4}{4!} \cdots
\]

Subtracting \( p_1 \) from \( p(t_0 + h) \), we get

\[
\frac{h^3}{3!}(-\frac{h^2}{12} g_{qqq} - \frac{h^2}{12} g_{qqq}g - \frac{h^2}{12} g_{qq}g - \cdots) = C_2 h^5
\]

This completes the second part of the proof.

As can be seen that, we find errors

\[
q(t_0 + h) - q_1 = C_1 h^5
\]

\[
p(t_0 + h) - p_1 = C_2 h^5
\]

So our new modified Lobatto method is a method of order 4.

4. Numerical Test Problem

4.1 Applications to Harmonic Oscillator System

We determine the modified differential equations based on the Lobatto IIIA–IIIB method for the linear Hamiltonian system, as an example of Harmonic Oscillation system. We then illustrate the trajectory of motion (phase space), energy error \( \| H(q,p) - H(q_0,p_0) \|_2 \) and global error \( \| y_{\text{exact}} - y_{\text{numeric}} \|_2 \) where \( y = y(q,p) \). The Hamiltonian of this system can be given as

\[
H(q,p) = \frac{1}{2} p^2 + \frac{1}{2} q^2
\]

so that the equations of motion become

\[
\dot{q} = H_p(q,p) = p
\]

\[
\dot{p} = H_q(q,p) = -q
\]
4.2 Modified Equations Based on Lobatto IIIA-IIIB Method

Harmonic oscillation problem can be read as

\[ \dot{q} = p = f(p) \]  
\[ \dot{p} = -q = -V_q(q) = g(q). \]  

(18)  
(19)

In this section we derive the modified differential equations of the system (18) and (19) based on Lobatto IIIA–IIIB methods. Applying (18) and (19) to the modified equations

\[ \begin{align*}
q' &= p + \frac{h^2}{6} g_q p = \left( I - \frac{h^2}{6} V_{qq} \right) p \\
p' &= -V_q(q) - \frac{h^2}{12}(g_{qq}(p,p) + g_q g)
\end{align*} \]

we obtain the modified differential equations of the system (18) and (19) in the form

\[ \begin{align*}
q' &= \left( 1 - \frac{h^2}{6} \right) p \\
p' &= -\left( 1 + \frac{h^2}{12} \right) q
\end{align*} \]  
(20)  
(21)

4.3 Numerical Implementation for Harmonic Oscillation

In this section we apply Lobatto IIIA–IIIB pair of order 2, Lobatto IIIA–IIIB pair of order 4, Runge Kutta method(order 4), Modified Midpoint method(order 4), Gauss Collocation method(order 4) to the system (18) and (19) and Modified Lobatto method of order 4 to the system (20) and (21) in order to show effectiveness. Comparison of these methods for \( p_{\text{initial}} = 1; q_{\text{initial}} = 0; h = .01; t = 0 : h : 100; n = \frac{100}{h} \) are illustrated in Figure 1 and 2 with respect to the energy error, global error. We observe that since all of these methods are symplectic, the shape of the trajectory preserved. Comparison of norm of global errors, norm of energy errors and CPU times for the methods we consider are illustrated in the Table 1.
Figure 1: Energy error and global error in Hamiltonian by 2-nd order Lobatto method, 4-th order Lobatto method and 4-th order Runge-Kutta method (from left to right).

### 4.4 Comparison of the norm of global error, norm of energy error and CPU time

<table>
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<th>METHODS</th>
<th>I</th>
<th>II</th>
<th>III</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lobatto method of order 4</td>
<td>0.0225</td>
<td>2.5342e-004</td>
<td>1.085</td>
</tr>
<tr>
<td>Runge Kutta method of order 4</td>
<td>3.4242e-007</td>
<td>4.0099e-009</td>
<td>0.577</td>
</tr>
<tr>
<td>Modified Midpoint of order 4</td>
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<td>0.733</td>
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<tr>
<td>Gauss Colloc. method of order 4</td>
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<td>1.6687e-013</td>
<td>2.366</td>
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<tr>
<td>Modi. Lobatto method of order 4</td>
<td>3.3803e-007</td>
<td>1.6428e-013</td>
<td>0.589</td>
</tr>
</tbody>
</table>

Table 1: Comparison of (I) the norm of global errors, (II) norm of energy errors and (III) CPU times in Hamiltonian

### 5. Conclusion

In the paper, we constructed 4-th order Modified Lobatto IIIA-IIIB pair method by using modified vector field idea. One can develop higher order method in the same manner. We showed that the consistency of the method and order of the method. From the simulation based on the harmonic oscillation problem the following results are revealed:
As the error of the methods we consider are increasing, the energy errors and global errors in solutions are decreasing.

Comparising of the 4th order methods showed that modified lobatto method is more efficient with respect to the energy errors, global errors and CPU times.

In future we will apply our method to nonlinear ODE and PDE problems.

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