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Starting algorithms for partitioned Runge-Kutta methods: the pair Lobatto IIIA-IIIB

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Abstract

Partitioned Runge-Kutta (PRK) methods are suitable for the numerical integration of separable Hamiltonian systems. For implicit PRK methods, the computational effort may be dominated by the cost of solving the non-linear systems. For these non-linear systems, good starting values minimize both the risk of a failed iteration and the effort required for convergence.

In this paper we consider the Lobatto IIIA-IIIB pair. Applying the theory developed by the authors for PRK methods, we obtain optimum predictors for this pair. Numerical experiments show the efficiency of these predictors.

Key words and expressions: Starting algorithms, stage value predictors, partitioned Runge-Kutta methods, Hamiltonian systems.

MSC: 65L05, 65L06, 65L80, 65H10.

1 Introduction

We consider partitioned differential equations of the form

$$\begin{cases} y' = f(y,z) & y(x_0) = y_0\,, \\ z' = g(y,z) & z(x_0) = z_0\,, \end{cases} \tag{1}$$

where $f : \mathbb{R}^l \times \mathbb{R}^m \longrightarrow \mathbb{R}^l$ and $g : \mathbb{R}^l \times \mathbb{R}^m \longrightarrow \mathbb{R}^m$ are sufficiently smooth functions.

An example of this type of systems are Hamiltonian systems

$$p' = -\frac{\partial H}{\partial q}\,, \tag{2}$$

$$q' = \frac{\partial H}{\partial p}\,, \tag{3}$$

where the Hamiltonian function H has the special structure

$$H(p,q) = T(p) + V(q)\,.$$

In this case, the Hamiltonian system (2)-(3) is of the form

$$\begin{aligned} p' &= f(q) \\ q' &= g(p) \end{aligned}$$

with $f = -\nabla_q V$, $g = \nabla_p T$.

For the numerical integration of (1) we consider partitioned Runge-Kutta (PRK) methods. The idea of the PRK methods is to take two different Runge-Kutta (RK) methods, $(\mathcal{A}, b, \hat{\mathcal{A}}, \hat{b})$, and to treat the variables y with the first method, $(\mathcal{A}, b)$, and the z variables with the second one, $(\hat{\mathcal{A}}, \hat{b})$. In this way, the numerical solution from (t_n, y_n, z_n) to $(t_{n+1}, y_{n+1}, z_{n+1})$ with the s-stage PRK method $(\mathcal{A}, b, \hat{\mathcal{A}}, \hat{b})$ is given by

$$\begin{aligned} y_{n+1} &= y_n + h\,(b^t \otimes I_l)\, f(Y_{n+1}, Z_{n+1})\,, \\ z_{n+1} &= z_n + h\,(\hat{b}^t \otimes I_m)\, g(Y_{n+1}, Z_{n+1})\,, \end{aligned}$$

where the internal stages vectors Y_{n+1}, Z_{n+1} are obtained from the system

$$Y_{n+1} = e \otimes y_n + h\,(\mathcal{A} \otimes I_l)\, f(Y_{n+1}, Z_{n+1})\,, \tag{4}$$

$$Z_{n+1} = e \otimes z_n + h\,(\hat{\mathcal{A}} \otimes I_m)\, g(Y_{n+1}, Z_{n+1})\,. \tag{5}$$

As usual, we have denoted by $\otimes$ the Kronecker product and by $e = (1, \ldots, 1)^t$. For implicit PRK methods, the computational effort may be dominated by the cost of solving the non-linear systems (4)-(5). These non-linear systems are solved with an iterative method that requires starting values $Y_{n+1}^{(0)}$, $Z_{n+1}^{(0)}$, and it is well known that these values must be as accurate as possible, because in other case, the number of iterations in each step may be too high or even worse, the convergence may fail.

A common way to proceed is to take as starting values the last computed numerical solution, i.e., $Y_{n+1}^{(0)} = e \otimes y_n$, $Z_{n+1}^{(0)} = e \otimes z_n$. We will refer to them as the trivial predictors. However it is also possible to involve the last computed internal stages, Y_n, Z_n, and the approximation y_{n-1}, and consider starting algorithms of the form

$$Y_{n+1}^{(0)} = b_0 \otimes y_{n-1} + (B \otimes I_l) Y_n\,, \tag{6}$$

$$Z_{n+1}^{(0)} = c_0 \otimes z_{n-1} + (C \otimes I_m) Z_n\,, \tag{7}$$

where b_0, $c_0 \in \mathbb{R}^s$, B and C are $s \times s$ matrices which have to be determined.

Several kinds of starting algorithms for RK methods, also called stage value predictors, have been studied by different authors ([16], [12], [14], [7], [4], [3], [5], [6], [1], [2]). The

starting algorithms considered for example in [16], [15] or [7] are of the form (6)-(7), whereas the ones considered for example in [12], [4] or [1] also involve function evaluations of the internal stages.

Although in this paper we only deal with Hamiltonian systems without restrictions (ODEs), we are also interested in Hamiltonian systems with restrictions (DAEs). For ODE systems we can use any of the stage value predictors mentioned in the previous paragraph, but this is not the case for DAEs. Predictors involving function evaluations cannot be used for this type of systems ([15], [8]). This is the reason why we use predictors of the form (6)-(7). These predictors have already been studied for PRK methods in [9].

In this paper we consider the PRK methods Lobatto IIIA-IIIB, that have been proved to be suitable ones for Hamiltonian systems ([10], [18]) and construct good starting algorithms for them. This is done in Section 2. The numerical experiments done in Section 3, show the efficiency of these starting algorithms.

2 Starting Algorithms for Lobatto IIIA-IIIB Methods

We consider the PRK methods $(\mathcal{A}, b, \hat{\mathcal{A}}, \hat{b})$, where $(\mathcal{A}, b)$ is the Lobatto IIIA method and $(\hat{\mathcal{A}}, \hat{b})$ is the Lobatto IIB method. We will refer to this PRK method as the Lobatto IIIA-IIB method. Observe that these methods share the same nodes, that is to say $c = \hat{c}$. Furthermore, the s-stage Lobatto IIIA method satisfies $C(s)$, and thus $\mathcal{A}c^{q-1} = c^q/q$, $q = 1, ..., s$; whereas the s-stage Lobatto IIIB method satisfies $C(s-2)$, and therefore $\hat{\mathcal{A}}\hat{c}^{q-1} = \hat{c}^q/q$, $q = 1, ..., s-2$.

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{5}{24} & \frac{1}{3} & \frac{-1}{24} \\
1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & \frac{1}{6} & \frac{-1}{6} & 0 \\
\frac{1}{2} & \frac{1}{6} & \frac{1}{3} & 0 \\
1 & \frac{1}{6} & \frac{5}{6} & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Figure 1: The pair Lobatto IIIA-IIIB for $s = 3$

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\frac{5-\sqrt{5}}{10} & \frac{11+\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & \frac{25-13\sqrt{5}}{120} & \frac{-1+\sqrt{5}}{120} \\
\frac{5+\sqrt{5}}{10} & \frac{11-\sqrt{5}}{120} & \frac{25+13\sqrt{5}}{120} & \frac{25+\sqrt{5}}{120} & \frac{-1-\sqrt{5}}{120} \\
1 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \\
\hline
 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
\qquad
\begin{array}{c|cccc}
0 & \frac{1}{12} & \frac{-1-\sqrt{5}}{24} & \frac{-1+\sqrt{5}}{24} & 0 \\
\frac{5-\sqrt{5}}{10} & \frac{1}{12} & \frac{25+\sqrt{5}}{120} & \frac{25-13\sqrt{5}}{120} & 0 \\
\frac{5+\sqrt{5}}{10} & \frac{1}{12} & \frac{25+13\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & 0 \\
1 & \frac{1}{12} & \frac{11-\sqrt{5}}{24} & \frac{11+\sqrt{5}}{24} & 0 \\
\hline
 & \frac{1}{16} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
$$

Figure 2: The pair Lobatto IIIA-IIIB for $s = 4$

In [9] the general order conditions for predictors of the form (6)-(7) have been obtained. Fortunately, these conditions are reduced considerably if the method PRK satisfies some simplifying assumptions, as it occurs with Lobatto IIIA-IIIB methods.

For $s \geq 3$, the s-stage Lobatto IIIA and IIIB methods satisfy at least $C(3)$ and $C(1)$ respectively. In this case, the general order conditions in [9] for the variable y are reduced to the following ones

$$\begin{aligned}
\text{Consistency:} \quad & b_0 + B\,e = e\,, \\
\text{Order 1:} \quad & B\,c = e + r\,c\,, \\
\text{Order 2:} \quad & B\,\mathcal{A}\,c = eb^t c + r\mathcal{A}(e + rc)\,, \\
\text{Order 3:} \quad & B\,\mathcal{A}c^2 = eb^t c^2 + r\mathcal{A}(e + rc)^2\,, \\
& B\,\mathcal{A}\hat{\mathcal{A}}c = eb^t \hat{\mathcal{A}}c + r\mathcal{A}eb^t c + r^2\mathcal{A}\hat{\mathcal{A}}(e + rc)\,,
\end{aligned} \tag{8}$$

whereas the order conditions for the variable z are reduced to

$$\begin{aligned}
\text{Consistency:} \quad & c_0 + C\,e = e\,, \\
\text{Order 1:} \quad & C\,c = e + r\,c\,, \\
\text{Order 2:} \quad & C\,\hat{\mathcal{A}}\,c = e\hat{b}^t c + r\hat{\mathcal{A}}(e + rc)\,, \\
\text{Order 3:} \quad & C\,\hat{\mathcal{A}}c^2 = e\hat{b}^t c^2 + r\hat{\mathcal{A}}(e + rc)^2\,, \\
& C\,\hat{\mathcal{A}}^2 c = e\hat{b}^t \hat{\mathcal{A}}c + r\hat{\mathcal{A}}e\hat{b}^t c + r^2\hat{\mathcal{A}}^2(e + rc)\,.
\end{aligned} \tag{9}$$

The parameter $r = h_{n+1}/h_n$, where h_{n+1} denotes the current stepsize, $h_{n+1} = t_{n+1} - t_n$, and h_n denotes the last stepsize, $h_n = t_n - t_{n-1}$.

For $s = 3$, if we take into account the number of parameters available and the number of order conditions, we get that the maximum order achieved is 2 for both variables, y and z. It is still possible to impose one of the two conditions of order 3, but not both of them.

For $s \geq 4$, the s-stage Lobatto IIIA and IIIB methods satisfy at least $C(4)$ and $C(2)$ respectively. Both of them satisfy $b^t c = \hat{b}^t c = 1/2$. In this case, in (8) and (9) the two conditions of order 3 are equivalent. Hence for $s = 4$, it is possible to achieve order 3 for both variables, y and z.

In order to simplify the implementation, it is interesting to initialize the variables y and z with the same coefficients. This situation corresponds to the case $b_0 = c_0$ and $B = C$ in (6)-(7).

In that case, for $s \geq 3$, up to order 2, the joint order conditions (8) and (9) are reduced to the following ones

$$\begin{aligned} \text{Consistency:} \quad & b_0 + B\,e = e\,, \\ \text{Order 1:} \quad & B\,c = e + r\,c\,, \\ \text{Order 2:} \quad & B\,\mathcal{A}\,c = eb^t c + r\mathcal{A}(e + rc)\,, \\ & B\,\hat{\mathcal{A}}\,c = e\hat{b}^t c + r\hat{\mathcal{A}}(e + rc)\,. \end{aligned}$$

Now it is easy to conclude that there exists a unique joint predictor of order 2 for the case $s = 3$. This predictor is given by the following coefficients

$$b_0 = \begin{pmatrix} -r^2 \\ r(3+2r) \\ r(6+5r) \end{pmatrix}\,, \quad B = \begin{pmatrix} r^2 & 0 & 1 \\ \frac{-1}{2}\,r(5+3r) & -r(2+r) & \frac{1}{2}\,(2+3r+r^2) \\ -r(5+3r) & -4r(1+r) & 1+3r+2r^2 \end{pmatrix}\,. \tag{10}$$

For $s \geq 4$, up to order 3, the joint order conditions (8) and (9) are reduced to the following ones

$$\begin{aligned} \text{Consistency:} \quad & b_0 + B\,e = e\,, \\ \text{Order 1:} \quad & B\,c = e + r\,c\,, \\ \text{Order 2:} \quad & B\,\mathcal{A}\,c = eb^t c + r\mathcal{A}(e + rc)\,, \\ \text{Order 3:} \quad & B\,\mathcal{A}c^2 = eb^t c^2 + r\mathcal{A}(e + rc)^2\,, \\ & B\,\hat{\mathcal{A}}c^2 = e\hat{b}^t c^2 + r\hat{\mathcal{A}}(e + rc)^2\,. \end{aligned}$$

We immediately obtain that for $s = 4$ there exists a unique joint predictor of order 3. This predictor is given by the following coefficients

$$b_0 = \begin{pmatrix} -1 - r^3 \\ -1 + \left(-6 + \frac{6}{\sqrt{5}}\right)\,r + 3\,\left(-3 + \sqrt{5}\right)\,r^2 + \left(-4 + \frac{9}{\sqrt{5}}\right)\,r^3 \\ -1 - \frac{6\left(5+\sqrt{5}\right)r}{5} - 3\,\left(3 + \sqrt{5}\right)\,r^2 + \left(-4 - \frac{9}{\sqrt{5}}\right)\,r^3 \\ -1 - 12\,r - 30\,r^2 - 19\,r^3 \end{pmatrix}\,, \tag{11}$$

$$B = \begin{pmatrix} 1+r^3 & 0 & 0 & 1 \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{pmatrix}\,, \tag{12}$$

where

$$
\begin{aligned}
b_{21} &= 1 - \frac{11\,\left(-5+\sqrt{5}\right)\,r}{10} - \frac{5\,\left(-3+\sqrt{5}\right)\,r^2}{2} + \left(3 - \frac{7}{\sqrt{5}}\right)\,r^3\,,\\
b_{22} &= \frac{\left(-5+3\,\sqrt{5}\right)\,r}{2} + \frac{\left(-9+5\,\sqrt{5}\right)\,r^2}{2} + \left(-2+\sqrt{5}\right)\,r^3\,,\\
b_{23} &= -\sqrt{5}\,r + \left(3-2\,\sqrt{5}\right)\,r^2 + \left(2-\sqrt{5}\right)\,r^3\,,\\
b_{24} &= 1 + \left(3 - \frac{3}{\sqrt{5}}\right)\,r + \left(3-\sqrt{5}\right)\,r^2 + \left(1 - \frac{2}{\sqrt{5}}\right)\,r^3\,,\\
b_{31} &= 1 + \frac{11\,\left(5+\sqrt{5}\right)\,r}{10} + \frac{5\,\left(3+\sqrt{5}\right)\,r^2}{2} + \left(3 + \frac{7}{\sqrt{5}}\right)\,r^3\,,\\
b_{32} &= \sqrt{5}\,r + \left(3+2\,\sqrt{5}\right)\,r^2 + \left(2+\sqrt{5}\right)\,r^3\,,\\
b_{33} &= \frac{\left(-5-3\,\sqrt{5}\right)\,r}{2} + \frac{\left(-9-5\,\sqrt{5}\right)\,r^2}{2} + \left(-2-\sqrt{5}\right)\,r^3\,,\\
b_{34} &= 1 + \left(3 + \frac{3}{\sqrt{5}}\right)\,r + \left(3+\sqrt{5}\right)\,r^2 + \left(1 + \frac{2}{\sqrt{5}}\right)\,r^3\,,\\
b_{41} &= 1 + 11\,r + 25\,r^2 + 14\,r^3\,,\\
b_{42} &= \frac{5\,\left(-1+\sqrt{5}\right)\,r}{2} + \frac{5\,\left(-1+3\,\sqrt{5}\right)\,r^2}{2} + 5\,\sqrt{5}\,r^3\,,\\
b_{43} &= \frac{-5\,\left(1+\sqrt{5}\right)\,r}{2} - \frac{5\,\left(1+3\,\sqrt{5}\right)\,r^2}{2} - 5\,\sqrt{5}\,r^3\,,\\
b_{44} &= 1 + 6\,r + 10\,r^2 + 5\,r^3\,.
\end{aligned}
$$

For Lobatto IIIA, the first stage of the variable y is explicit. As $Y_{n,1} = y_{n-1}$ and $Y_{n,s} = y_n$, in (10) and (11)-(12) we get $Y_1^{(0)} = y_n$, and therefore, as expected, the first stage of the variable y is not initialized. Observe that this is not the case for Lobatto IIIB method. In this case the first stage is implicit and the coefficients in (10) and (11)-(12) are necessary to obtain a predictor.

3 Numerical Experiments

In this section we test the predictor constructed in the previous section for the 3-stage pair Lobatto IIIA-IIIB. We have selected an academic problem and the well known restricted three-body problem.

In both cases we have proceeded in the same way. The stopping criteria for the Newton iterations is

$$\frac{||\Delta Y^{(k)}||}{||Y^{(k)}||} \leq TOL\,.$$

The problems have been integrated for different values of TOL and for different stepsizes. In Tables 1-6 we show the average number of iterations per step needed when the trivial predictor is used, and the ones when the optimum predictor given by (10) is used. For each value of TOL and h, the values on the left correspond to the trivial predictor, whereas the values on the right correspond to the optimum predictor given by (10).

3.1 Problem 1

The problem is given by

$$\begin{cases} y' = 4(z+t)^2 + 2t - 2 & y(0) = 0 \\ z' = -\frac{y-t^2}{2(z+t)} - 1 & z(0) = 1 \end{cases} \tag{13}$$

The exact solution is $y(t) = \sin t + t\,,\ z(t) = \cos t - t$. We have integrated this problem for $t \in [0, 1]$.

TOL / h	1.0E-3	1.0E-5	1.0E-7
1.0E-2	2.000/1.010	2.000/1.190	3.000/2.010
5.0E-3	2.000/1.005	2.000/1.005	2.555/2.005
2.5E-3	2.000/1.002	2.000/1.002	2.000/2.000
1.0E-3	1.898/1.001	2.000/1.001	2.000/1.192

Table 1: Iterations per step. Problem 1

It can be seen that except in one case, the number of iterations is lower with the predictor constructed in this paper. The exception is for $h = 2.5\text{E-}03$ and $TOL = 1.0\text{E-}7$ where the number of iterations coincides. We remark that in this case, the numerical solution obtained with the optimum predictor is more accurate.

3.2 The restricted three-body problem

We have considered the restricted three-body problem from [13]

$$\begin{cases} x' = v_x & x(0) = x_0 \\ y' = v_y & y(0) = y_0 \\ z' = v_z & z(0) = z_0 \\ v_x' = 2\,v_y + x - \left[\mu_1 \frac{x+\mu_2}{r_1^3} + \mu_2 \frac{x-\mu_1}{r_2^3}\right] & v_x(0) = v_{x0} \\ v_y' = -2\,v_x + y - \left[\frac{\mu_1}{r_1^3} + \frac{\mu_2}{r_2^3}\right] y & v_y(0) = v_{y0} \\ v_z' = -\left[\frac{\mu_1}{r_1^3} + \frac{\mu_2}{r_2^3}\right] z & v_z(0) = v_{z0} \end{cases} \tag{14}$$

where $\mu_2 = 1 - \mu_1$, and

$$r_1 = \sqrt{(x+\mu_2)^2 + y^2 + z^2} \qquad r_2 = \sqrt{(x-\mu_1)^2 + y^2 + z^2}\,.$$

We have integrated this problem for $t \in [0, 5]$ with different values of the parameter μ_1 and different initial conditions.

Case I

We take $\mu_1 = 0.8$ and the initial values $(0.45, 0, 0, 0, 0, 0)$. The numerical results are shown in Table 2.

TOL / h	1.0E-3	1.0E-5	1.0E-7
1.0E-2	2.112/1.284	2.542/1.130	3.090/2.436
5.0E-3	2.028/1.103	2.300/1.802	2.874/2.187
2.5E-3	2.005/1.026	2.136/1.492	2.560/2.056
1.0E-3	1.913/1.000	2.026/1.206	2.277/1.938

Table 2: Iterations per step: $\mu_1 = 0.8$

Case II

We take $\mu_1 = 0.95$ and the initial values $(0.45, 0, 0, 0, 1.199, 0.11)$. The numerical results are shown in Table 3.

TOL / h	1.0E-3	1.0E-5	1.0E-7
1.0E-2	2.026/1.050	2.094/1.400	2.540/2.074
5.0E-3	2.010/1.023	2.049/1.123	2.296/2.036
2.5E-3	2.004/1.011	2.025/ 1.061	2.091/2.015
1.0E-3	1.291/1.000	2.010/ 1.030	2.042/1.317

Table 3: Iterations per step: $\mu_1 = 0.95$

Case III

We take $\mu_1 = 0.999046125$ and the initial values $(-1.02745, 0, 0, 0, 0.04032, 0)$. The numerical results are shown in Table 4.

TOL / h	1.0E-5	1.0E-7	1.0E-9
1.0E-2	2.000/1.002	2.000/1.002	2.000/1.066
5.0E-3	2.000/1.001	2.000/1.001	2.000/1.001
2.5E-3	2.000/1.000	2.000/ 1.001	2.000/1.000
1.0E-3	2.000/1.000	2.000/ 1.000	2.000/1.000

Table 4: Iterations per step: $\mu_1 = 0.999046125$

In Tables 2-4 we again see that the number of iterations needed when we use the predictors constructed in this paper is lower than the ones needed when the trivial predictor is used.

We remark that the reduction in the number of iterations when solving the non-linear systems implies a reduction in the total CPU time needed for the numerical integration, and hence it may be essential when long time integrations are done.

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