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ORDER CONDITIONS FOR PARTITIONED RUNGE-KUTTA METHODS

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Abstract. We illustrate the use of the recent approach by P. Albrecht to the derivation of order conditions for partitioned Runge-Kutta methods for ordinary differential equations.

Keywords: Partitioned Runge-Kutta method, ordinary differential equation, order conditions

MSC 2000: 65L05, 65L06

Introduction

Consider a partitioned system of ordinary differential equations (ODEs)

$$\begin{cases} p' = f^p(t,p,q), \\ q' = f^q(t,p,q), \end{cases} \tag{1.1}$$

$t \in [t_0, T]$, $p \in \mathbb{R}^{d_1}$, $q \in \mathbb{R}^{d_2}$, where the functions f^p and f^q are sufficiently smooth. Such systems are encountered in many practical applications. Typical examples are second order differential equations $y'' = f(t,y,y')$ which by putting $p = y$ and $q = y'$ can be written in the form

$$\begin{cases} p' = q, \\ q' = f(t,p,q); \end{cases}$$

Hamiltonian systems

$$\begin{cases} p' = -\dfrac{\partial H}{\partial q}, \\ q' = +\dfrac{\partial H}{\partial p}, \end{cases}$$

where $d_1 = d_2 = d$ is the number of the degrees of freedom, p are generalized coordinates, q are generalized momenta, and H is the Hamiltonian (total energy of the system); and singular perturbation problems

$$\begin{cases} y' = f(y, z), \\ \varepsilon z' = g(y, z), \end{cases}$$

where ε is a small parameter. The Volterra integral equation of the second kind

$$y(t) = g(t) + \int_{t_0}^{t} k\big(t, s, y(s)\big) ds,$$

$t \in [t_0, T]$, can also be written as an infinite system of partitioned ODEs as demonstrated by Brunner, Hairer and Nørsett [4].

The system (1.1) will be solved by the partitioned Runge-Kutta (PRK) method

$$\begin{cases} P_i = p_n + h \sum_{j=1}^{s} a_{ij} f^p(t_{n+c_j}, P_j, Q_j), \\ Q_i = q_n + h \sum_{j=1}^{s} \tilde{a}_{ij} f^q(t_{n+\tilde{c}_j}, P_j, Q_j), \\ p_{n+1} = p_n + h \sum_{i=1}^{s} b_i f^p(t_{n+c_i}, P_i, Q_i), \\ q_{n+1} = q_n + h \sum_{i=1}^{s} \tilde{b}_i f^q(t_{n+\tilde{c}_i}, P_i, Q_i), \end{cases} \tag{1.2}$$

$i = 1, 2, \ldots, s$, $n = 0, 1, \ldots, N-1$, $Nh = T - t_0$, where the coefficients c_i, a_{ij}, b_i, and $\tilde{c}_i$, $\tilde{a}_{ij}$, $\tilde{b}_i$, $c_i = \sum_{j=1}^{s} a_{ij}$, $\tilde{c}_i = \sum_{j=1}^{s} \tilde{a}_{ij}$ represent two different RK schemes. They will be represented by two tables

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccc} c_1 & a_{11} & \ldots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \ldots & a_{ss} \\ \hline & b_1 & \ldots & b_s \end{array}, \qquad \begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b}^T \end{array} = \begin{array}{c|ccc} \tilde{c}_1 & \tilde{a}_{11} & \ldots & \tilde{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{c}_s & \tilde{a}_{s1} & \ldots & \tilde{a}_{ss} \\ \hline & \tilde{b}_1 & \ldots & \tilde{b}_s \end{array}.$$

Hairer [6] (see also [7]) developed a theory of P-series to study order conditions for (1.2). As observed in [7] the derivation of order conditions simplifies considerably if we assume that $c = \tilde{c}$. The resulting order conditions in this case up to the order $r = 4$ have been listed in Griepentrog [5]. However, in many practical applications it is important to consider methods with $c \neq \tilde{c}$. This is the case, for example, when integrating separable Hamiltonian systems, i.e., systems for which the Hamiltonian H has the special structure

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

In applications to mechanics T and V would represent the kinetic and the potential energy of the system, respectively. It is known (see for example [11]) that such systems can be efficiently integrated by symplectic PRK methods which are also effectively explicit. These methods have the form

$$\begin{array}{c|ccccc} 0 & 0 & 0 & 0 & \dots & 0 \\ c_2 & b_1 & 0 & 0 & \dots & 0 \\ c_3 & b_1 & b_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & b_1 & b_2 & b_3 & \dots & 0 \\ \hline & b_1 & b_2 & b_3 & \dots & b_s \end{array}, \qquad \begin{array}{c|ccccc} \tilde{c}_1 & \tilde{b}_1 & 0 & 0 & \dots & 0 \\ \tilde{c}_2 & \tilde{b}_1 & \tilde{b}_2 & 0 & \dots & 0 \\ \tilde{c}_3 & \tilde{b}_1 & \tilde{b}_2 & \tilde{b}_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \tilde{c}_s & \tilde{b}_1 & \tilde{b}_2 & \tilde{b}_3 & \dots & \tilde{b}_s \\ \hline & \tilde{b}_1 & \tilde{b}_2 & \tilde{b}_3 & \dots & \tilde{b}_s \end{array},$$

$c_i = \sum_{j=1}^{i-1} b_j$, $\tilde{c}_i = \sum_{j=1}^{i} \tilde{b}_j$, $i = 1, 2, \dots, s$, hence, in general, $c \neq \tilde{c}$.

It is the purpose of this paper to derive order conditions for PRK methods with $c \neq \tilde{c}$ using the alternative approach to the order theory developed by Albrecht [2], [3]. This approach was also used to derive order conditions for Rosenbrock methods by Albrecht [2], for constant and variable two-step RK methods by Jackiewicz and Tracogna [9], [10], and for a certain class of general linear methods by Jackiewicz and Vermiglio [8].

As in the case of the approach based on the P-series [6], [7], Albrecht's approach also simplifies considerably for PRK methods with $c = \tilde{c}$.

2. General order condition

Introducing the notation

$$\begin{aligned} P &= [P_1, \dots, P_s]^T, & Q &= [Q_1, \dots, Q_s]^T, \\ t_{n+c} &= [t_{n+c_1}, \dots, t_{n+c_s}]^T, & t_{n+c_i} &= t_n + c_i h, \\ t_{n+\tilde{c}} &= [t_{n+\tilde{c}_1}, \dots, t_{n+\tilde{c}_s}]^T, & t_{n+\tilde{c}_i} &= t_n + \tilde{c}_i h, \end{aligned}$$

$$\begin{aligned} f^p(t_{n+c}, P, Q) &= [f^p(t_{n+c_1}, P_1, Q_1), \dots, f^p(t_{n+c_s}, P_s, Q_s)]^T, \\ f^q(t_{n+\tilde{c}}, P, Q) &= [f^q(t_{n+\tilde{c}_1}, P_1, Q_1), \dots, f^q(t_{n+\tilde{c}_s}, P_s, Q_s)]^T, \\ e &= [1, \dots, 1]^T \in \mathbb{R}^s, \end{aligned}$$

the method (1.2) can be written in the matrix form

$$\begin{cases} P = p_n e + hAf^p(t_{n+c}, P, Q), \\ Q = q_n e + h\tilde{A} f^q(t_{n+\tilde{c}}, P, Q), \\ p_{n+1} = p_n + hb^T f^p(t_{n+c}, P, Q), \\ q_{n+1} = q_n + h\tilde{b}^T f^q(t_{n+\tilde{c}}, P, Q), \end{cases}$$

$n = 0, 1, \ldots, N-1$. We define the local discretization errors hd^p_{n+c}, $hd^q_{n+\tilde{c}}$, $h\hat{d}^p_{n+1}$, $h\hat{d}^q_{n+1}$ of stage values P, Q, and the last stages p_{n+1}, q_{n+1} as residua obtained by replacing in (2.1) the values P, Q by $p(t_{n+c})$, $q(t_{n+\tilde{c}})$ and p_{n+1}, q_{n+1} by $p(t_{n+1})$, $q(t_{n+1})$, where

$$\begin{cases} p(t_{n+c}) = [p(t_{n+c_1}), \ldots, p(t_{n+c_s})]^T, \\ q(t_{n+\tilde{c}}) = [q(t_{n+\tilde{c}_1}), \ldots, q(t_{n+\tilde{c}_s})]^T. \end{cases}$$

This leads to

$$\begin{cases} p(t_{n+c}) = p(t_n)e + hAf^p\big(t_{n+c}, p(t_{n+c}), q(t_{n+\tilde{c}})\big) + hd^p_{n+c}, \\ q(t_{n+\tilde{c}}) = q(t_n)e + h\tilde{A}f^q\big(t_{n+\tilde{c}}, p(t_{n+c}), q(t_{n+\tilde{c}})\big) + hd^q_{n+\tilde{c}}, \\ p(t_{n+1}) = p(t_n) + hb^T f^p\big(t_{n+c}, p(t_{n+c}), q(t_{n+\tilde{c}})\big) + h\hat{d}^p_{n+1}, \\ q(t_{n+1}) = q(t_n) + h\tilde{b}^T f^q\big(t_{n+\tilde{c}}, p\big(t_{n+c}), q(t_{n+\tilde{c}})\big) + h\hat{d}^q_{n+1}, \end{cases} \tag{2.2}$$

$n = 0, 1, \ldots, N-1$. Putting

$$\xi^p_{n+c} = p(t_{n+c}) - P, \qquad \hat{\xi}^p_{n+1} = p(t_{n+1}) - p_{n+1},$$

$$\xi^q_{n+\tilde{c}} = q(t_{n+\tilde{c}}) - Q, \qquad \hat{\xi}^q_{n+1} = q(t_{n+1}) - q_{n+1},$$

$$\eta^p_{n+c} = f^p\big(t_{n+c}, p(t_{n+c}), q(t_{n+\tilde{c}})\big) - f^p(t_{n+c}, P, Q),$$

$$\eta^q_{n+\tilde{c}} = f^q\big(t_{n+\tilde{c}}, p(t_{n+c}), q(t_{n+\tilde{c}})\big) - f^q(t_{n+\tilde{c}}, P, Q)$$

and subtracting (2.1) from (2.2) we obtain

$$\begin{aligned} \xi^p_{n+c} &= \hat{\xi}^p_n e + hA\eta^p_{n+c} + hd^p_{n+c}, \\ \xi^q_{n+\tilde{c}} &= \hat{\xi}^q_n e + h\tilde{A}\eta^q_{n+\tilde{c}} + hd^q_{n+\tilde{c}}, \\ \hat{\xi}^p_{n+1} &= \hat{\xi}^p_n + hb^T\eta^p_{n+c} + h\hat{d}^p_{n+1} \\ &= \hat{\xi}^p_{n-1} + hb^T\eta^p_{n-1+c} + h\hat{d}^p_n + hb^T\eta^p_{n+c} + h\hat{d}^p_{n+1} \\ &= \ \ldots \ = h\sum_{l=0}^{n} \hat{d}^p_{l+1} + hb^T\sum_{l=0}^{n}\eta^p_{l+c}, \\ \hat{\xi}^q_{n+1} &= \hat{\xi}^q_n + h\tilde{b}^T\eta^q_{n+\tilde{c}} + h\hat{d}^q_{n+1} \\ &= \hat{\xi}^q_{n-1} + h\tilde{b}^T\eta^q_{n-1+\tilde{c}} + h\hat{d}^q_n + h\tilde{b}^T\eta^q_{n+\tilde{c}} + h\hat{d}^q_{n+1} \\ &= \ \ldots \ = h\sum_{l=0}^{n} \hat{d}^q_{l+1} + h\tilde{b}^T\sum_{l=0}^{n}\eta^q_{l+\tilde{c}} \end{aligned}$$

since $\hat{\xi}_0^p = p(t_0) - p_0 = 0$ and $\hat{\xi}_0^q = q(t_0) - q_0 = 0$. The above relations lead to the following general order condition for PRK method (2.1).

Theorem 2.1. *Assume that the external stages p_{n+1} and q_{n+1} of the* PRK *method* (2.1) *have order of consistency $r \geqslant 3$, i.e., $\hat{d}_n^p = O(h^r)$ and $\hat{d}_n^q = O(h^r)$, $n = 0, 1, \ldots, N$. Then the* PRK *method* (2.1) *converges with order r, i.e., $\hat{\xi}_n^p = O(h^r)$ and $\hat{\xi}_n^q = O(h^r)$, $n = 0, 1, \ldots, N$, if and only if*

$$\begin{cases} b^T \eta_{n+c}^p & = O(h^r), \\ \tilde{b}^T \eta_{n+\tilde{c}}^q & = O(h^r), \end{cases} \tag{2.3}$$

$n = 0, 1, \ldots, N-1$. Moreover, the global errors ξ_{n+c}^p and $\xi_{n+\tilde{c}}^q$ of the internal stages P and Q are given by

$$\begin{cases} \xi_{n+c}^p = & h d_{n+c}^p + hA\eta_{n+c}^p + O(h^r), \\ \xi_{n+\tilde{c}}^q = & h d_{n+\tilde{c}}^q + h\tilde{A}\eta_{n+\tilde{c}}^q + O(h^r), \end{cases} \tag{2.4}$$

$n = 0, 1, \ldots, N-1$, where hd_{n+c}^p and $hd_{n+\tilde{c}}^q$ are defined in (2.2).

P r o o f. It follows from the assumptions of the theorem and from (2.3) that $\hat{\xi}_{n+1}^p = O(h^r)$ and $\hat{\xi}_{n+1}^q = O(h^r)$, which means convergence of order r. Substituting the above relations into the formulas for ξ_{n+c}^p and $\xi_{n+\tilde{c}}^q$ we obtain (2.4). $\square$

The order conditions (2.3) are not convenient to use since they depend on the functions f^p and f^q appearing in (1.1) (through η_{n+c}^p and $\eta_{n+\tilde{c}}^q$). In the rest of the paper we will reformulate (2.3) in terms of the coefficients c, A, b, and $\tilde{c}$, $\tilde{A}$, $\tilde{b}$ of PRK method (2.1).

3. Reformulation of order conditions for PRK methods

The following technical lemma expresses η_{n+c}^p and $\eta_{n+\tilde{c}}^q$ in terms of ξ_{n+c}^p and $\xi_{n+\tilde{c}}^q$. This lemma will be instrumental in expressing order conditions (2.3) in a more convenient form.

Lemma 3.1. *Assume that the functions p and q are sufficiently smooth. Then*

$$(3.1)\quad \begin{cases} \eta^p_{n+c} = & \displaystyle\sum_{l=1}^{\infty}\sum_{\nu=1}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=1}^{\infty}\frac{1}{\mu!}G^p_{l\nu\mu}(t_n) \\ & \displaystyle\times\Big(\sum_{j=1}^{\infty}\frac{1}{j!}q^{(j)}(t_n)(\widetilde{D}-D)^j h^j\Big)^{\mu}(\xi^p_{n+c})^{l-\nu}(\xi^q_{n+\tilde{c}})^{\nu}, \\ \eta^q_{n+\tilde{c}} = & \displaystyle\sum_{l=1}^{\infty}\sum_{\nu=1}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=1}^{\infty}\frac{1}{\mu!}G^q_{l\nu\mu}(t_n) \\ & \displaystyle\times\Big(\sum_{j=1}^{\infty}\frac{1}{j!}p^{(j)}(t_n)(D-\widetilde{D})^j h^j\Big)^{\mu}(\xi^p_{n+c})^{l-\nu}(\xi^q_{n+\tilde{c}})^{\nu} \end{cases}$$

with

$$(3.2)\quad \begin{cases} G^p_{l\nu\mu}(t) := \mathrm{diag}\big(g^p_{l\nu\mu}(t+c_1h),\dots,g^p_{l\nu\mu}(t+c_sh)\big) \\ \qquad = g^p_{l\nu\mu}(t)I + hD(g^p_{l\nu\mu})'(t) + \frac{1}{2}h^2D^2(g^p_{l\nu\mu})''(t)+\dots, \\ G^q_{l\nu\mu}(t) := \mathrm{diag}\big(g^q_{l\nu\mu}(t+c_1h),\dots,g^q_{l\nu\mu}(t+c_sh)\big) \\ \qquad = g^q_{l\nu\mu}(t)I + h\widetilde{D}(g^q_{l\nu\mu})'(t) + \frac{1}{2}h^2\widetilde{D}^2(g^q_{l\nu\mu})''(t)+\dots, \end{cases}$$

where

$$(3.3)\quad \begin{cases} g^p_{l\nu\mu}(t) := \dfrac{\partial^{l+\mu}f^p}{\partial p^{l-\nu}\partial q^{\nu+\mu}}\big(t,p(t),q(t)\big), \\ g^q_{l\nu\mu}(t) := \dfrac{\partial^{l+\mu}f^q}{\partial p^{l-\nu+\mu}\partial q^{\nu}}\big(t,p(t),q(t)\big) \end{cases}$$

and

$$D = \mathrm{diag}(c_1,\dots,c_s), \qquad \tilde{D} = \mathrm{diag}(\tilde{c}_1,\dots,\tilde{c}_s).$$

P r o o f. Expanding $f^p(t_{n+c_i},P_i,Q_i)$ and $f^q(t_{n+\tilde{c}_i},P_i,Q_i)$ into Taylor series around $\big(t_{n+c_i},p(t_{n+c_i}),q(t_{n+\tilde{c}_i})\big)$ and $\big(t_{n+\tilde{c}_i},p(t_{n+c_i}),q(t_{n+\tilde{c}_i})\big)$, respectively, we obtain

$$\begin{aligned} \eta^p_{n+c_i} &= \sum_{l=1}^{\infty}\sum_{\nu=0}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=0}^{\infty}\frac{1}{\mu!}g^p_{l\nu\mu}(t_{n+c_i}) \\ &\quad\times\big(q(t_{n+\tilde{c}_i})-q(t_{n+c_i})\big)^{\mu}(\xi^p_{n+c_i})^{l-\nu}(\xi^q_{n+\tilde{c}_i})^{\nu}, \\ \eta^q_{n+\tilde{c}_i} &= \sum_{l=1}^{\infty}\sum_{\nu=0}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=0}^{\infty}\frac{1}{\mu!}g^q_{l\nu\mu}(t_{n+\tilde{c}_i}) \\ &\quad\times\big(p(t_{n+c_i})-p(t_{n+\tilde{c}_i})\big)^{\mu}(\xi^p_{n+c_i})^{l-\nu}(\xi^q_{n+\tilde{c}_i})^{\nu}, \end{aligned}$$

where $g^p_{l\nu\mu}$ and $g^q_{l\nu\mu}$ are defined by (3.3). Substituting

$$q(t_{n+\tilde{c}_i}) - q(t_{n+c_i}) = \sum_{j=1}^{\infty} \frac{1}{j!} q^{(j)}(t_n)(\tilde{c}_i - c_i)^j h^j$$

and

$$p(t_{n+c_i}) - p(t_{n+\tilde{c}_i}) = \sum_{j=1}^{\infty} \frac{1}{j!} p^{(j)}(t_n)(c_i - \tilde{c}_i)^j h^j$$

into $\eta^p_{n+c_i}$ and $\eta^q_{n+\tilde{c}_i}$ we obtain formulas which are equivalent to (3.1) with $G^p_{l\nu\mu}$ and $G^q_{l\nu\mu}$ defined by (3.2). □

Using the notation employed in the above lemma the local discretization errors hd^p_{n+c}, $hd^q_{n+\tilde{c}}$, $h\hat{d}^p_{n+1}$ and $h\hat{d}^q_{n+1}$ appearing in (2.2) of the PRK method (2.1) can be written in the form

$$(3.4) \quad \begin{cases} hd^p_{n+c} = & \displaystyle\sum_{l=1}^{r+1} \gamma^p_l h^l p^{(l)}(t_n) \\ & \displaystyle -hA \sum_{\mu=1}^{\infty} \frac{1}{\mu!} G^p_{00\mu}(t_n) \left(\sum_{j=1}^{\infty} \frac{1}{j!} q^{(j)}(t_n)(\tilde{c} - c)^j h^j \right)^{\mu} \\ & +O(h^{r+2}), \\ hd^q_{n+\tilde{c}} = & \displaystyle\sum_{l=1}^{r+1} \gamma^q_l h^l q^{(l)}(t_n) \\ & \displaystyle -h\tilde{A} \sum_{\mu=1}^{\infty} \frac{1}{\mu!} G^q_{00\mu}(t_n) \left(\sum_{j=1}^{\infty} \frac{1}{j!} p^{(j)}(t_n)(c - \tilde{c})^j h^j \right)^{\mu} \\ & +O(h^{r+2}), \end{cases}$$

$$(3.5) \quad \begin{cases} h\hat{d}^p_{n+1} = & \displaystyle\sum_{l=1}^{r+1} \hat{\gamma}^p_l h^l p^{(l)}(t_n) \\ & \displaystyle -hb^T \sum_{\mu=1}^{\infty} \frac{1}{\mu!} G^p_{00\mu}(t_n) \left(\sum_{j=1}^{\infty} \frac{1}{j!} q^{(j)}(t_n)(\tilde{c} - c)^j h^j \right)^{\mu} \\ & +O(h^{r+2}), \\ h\hat{d}^q_{n+1} = & \displaystyle\sum_{l=1}^{r+1} \hat{\gamma}^q_l h^l q^{(l)}(t_n) \\ & \displaystyle -h\tilde{b}^T \sum_{\mu=1}^{\infty} \frac{1}{\mu!} G^q_{00\mu}(t_n) \left(\sum_{j=1}^{\infty} \frac{1}{j!} p^{(j)}(t_n)(c - \tilde{c})^j h^j \right)^{\mu} \\ & +O(h^{r+2}), \end{cases}$$

where

$$\gamma_l^p := \frac{c^l}{l!} - A\frac{c^{l-1}}{(l-1)!}, \qquad \gamma_l^q := \frac{\tilde{c}^l}{l!} - \tilde{A}\frac{\tilde{c}^{l-1}}{(l-1)!},$$
$$\hat{\gamma}_l^p := \frac{1}{l!} - b^T\frac{c^{l-1}}{(l-1)!}, \qquad \hat{\gamma}_l^q := \frac{1}{l!} - \tilde{b}^T\frac{\tilde{c}^{l-1}}{(l-1)!},$$

$l = 1, 2, \ldots$.

Define functions u^p, u^q, v^p and v^q by

$$\begin{aligned}
u^p &:= \xi_{n+c}^p - hd_{n+c}^p - hA\eta_{n+c}^p + O(h^r),\\
u^q &:= \xi_{n+\tilde{c}}^q - hd_{n+\tilde{c}}^q - h\tilde{A}\eta_{n+\tilde{c}}^q + O(h^r),\\
v^p &:= \eta_{n+c}^p - \sum_{l=1}^{\infty}\sum_{\nu=1}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=1}^{\infty}\frac{1}{\mu!}G_{l\nu\mu}^p(t_n)\\
&\quad\times\left(\sum_{j=1}^{\infty}\frac{1}{j!}q^{(j)}(t_n)(\widetilde{D}-D)^j h^j\right)^{\mu}(\xi_{n+c}^p)^{l-\nu}(\xi_{n+\tilde{c}}^q)^{\nu},\\
v^q &:= \eta_{n+\tilde{c}}^q - \sum_{l=1}^{\infty}\sum_{\nu=1}^{l}\frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu}\sum_{\mu=1}^{\infty}\frac{1}{\mu!}G_{l\nu\mu}^q(t_n)\\
&\quad\times\left(\sum_{j=1}^{\infty}\frac{1}{j!}p^{(j)}(t_n)(D-\widetilde{D})^j h^j\right)^{\mu}(\xi_{n+c}^p)^{l-\nu}(\xi_{n+\tilde{c}}^q)^{\nu}.
\end{aligned}$$

These functions are analytical at $\xi_{n+c}^p = 0$, $\xi_{n+\tilde{c}}^q = 0$, $\eta_{n+c}^p = 0$, $\eta_{n+\tilde{c}}^q = 0$ and $h = 0$, moreover

$$\det\begin{bmatrix}
\dfrac{\partial u^p}{\partial \xi_{n+c}^p} & \dfrac{\partial u^p}{\partial \xi_{n+\tilde{c}}^q} & \dfrac{\partial u^p}{\partial \eta_{n+c}^p} & \dfrac{\partial u^p}{\partial \eta_{n+\tilde{c}}^q}\\
\dfrac{\partial u^q}{\partial \xi_{n+c}^p} & \dfrac{\partial u^q}{\partial \xi_{n+\tilde{c}}^q} & \dfrac{\partial u^q}{\partial \eta_{n+c}^p} & \dfrac{\partial u^q}{\partial \eta_{n+\tilde{c}}^q}\\
\dfrac{\partial v^p}{\partial \xi_{n+c}^p} & \dfrac{\partial v^p}{\partial \xi_{n+\tilde{c}}^q} & \dfrac{\partial v^p}{\partial \eta_{n+c}^p} & \dfrac{\partial v^p}{\partial \eta_{n+\tilde{c}}^q}\\
\dfrac{\partial v^q}{\partial \xi_{n+c}^p} & \dfrac{\partial v^q}{\partial \xi_{n+\tilde{c}}^q} & \dfrac{\partial v^q}{\partial \eta_{n+c}^p} & \dfrac{\partial v^q}{\partial \eta_{n+\tilde{c}}^q}
\end{bmatrix}_{|(\xi_{n+c}^p,\xi_{n+\tilde{c}}^q,\eta_{n+c}^p,\eta_{n+\tilde{c}}^q,h)=(0,0,0,0,0)}$$
$$= \det\begin{bmatrix}
I & 0 & 0 & 0\\
0 & I & 0 & 0\\
-G_{100}^p & -G_{110}^q & I & 0\\
-G_{100}^q & -G_{110}^q & 0 & I
\end{bmatrix} = 1.$$

Therefore, it follows from the implicit function theorem that the system of equations

$$u^p = 0, \quad u^q = 0, \quad v^p = 0, \quad v^q = 0$$

has a unique solution $(\xi^p_{n+c}, \xi^q_{n+\tilde{c}}, \eta^p_{n+c}, \eta^q_{n+\tilde{c}})$ around $h = 0$. This solution can be expanded into the Taylor series of the form

$$\tag{3.6} \begin{cases} \xi^p_{n+c} = s^p_2(t_n)h^2 + s^p_3(t_n)h^3 + \ldots + s^p_{r-1}(t_n)h^{r-1} + O(h^r), \\ \xi^q_{n+\tilde{c}} = s^q_2(t_n)h^2 + s^q_3(t_n)h^3 + \ldots + s^q_{r-1}(t_n)h^{r-1} + O(h^r), \end{cases}$$

and

$$\tag{3.7} \begin{cases} \eta^p_{n+c} = w^p_2(t_n)h^2 + w^p_3(t_n)h^3 + \ldots + w^p_{r-1}(t_n)h^{r-1} + O(h^r), \\ \eta^q_{n+\tilde{c}} = w^q_2(t_n)h^2 + w^q_3(t_n)h^3 + \ldots + w^q_{r-1}(t_n)h^{r-1} + O(h^r). \end{cases}$$

The fact that the above expressions start with terms of order $O(h^2)$ follows from the definitions of ξ^p_{n+c}, $\xi^q_{n+\tilde{c}}$, η^p_{n+c} and $\eta^q_{n+\tilde{c}}$.

Using the formulas for $h\hat{d}^p_{n+1}$, $h\hat{d}^q_{n+1}$ (compare (3.5)) and the expressions (3.7) we can reformulate Theorem 2.1 in a more convenient form as follows.

Theorem 3.2. *The* PRK *method* (2.1) *has order* r *if and only if* $\hat{d}^p_n = O(h^r)$, $\hat{d}^q_n = O(h^r)$, $n = 0, 1, \ldots, N$, *and*

$$\tag{3.8} \begin{cases} b^T w^p_i = O(h^r), \\ \tilde{b}^T w^q_i = O(h^r), \end{cases}$$

$i = 2, 3, \ldots, r-1$.

4. Recursive generation of order conditions

We will need the multinomial formula

$$\tag{4.1} \left(\sum_{k=1}^{\infty} \frac{x_k}{k!} t^k\right)^m = m! \sum_{n=m}^{\infty} \frac{t^n}{n!} \sum_{\substack{a_1+2a_2+\ldots+na_n=n \\ a_1+a_2+\ldots+a_n=m}} (n; a_1, a_2, \ldots, a_n)' x_1^{a_1} x_2^{a_2} \ldots x_n^{a_n},$$

where

$$(n; a_1, a_2, \ldots, a_n)' := \frac{n!}{(1!)^{a_1} a_1! (2!)^{a_2} a_2! \ldots (n!)^{a_n} a_n!},$$

compare [1], page 823.

We have the following theorem.

Theorem 4.1. *The vectors r_i^p, r_i^q, w_i^p, and w_i^q appearing in* (3.6) *and* (3.7) *satisfy the recursions*

$$r_i^p = \gamma_i^p p^{(i)} + Aw_{i-1}^p - \sum_{\mu=1}^{\infty} \sum_{\substack{\delta+\gamma+1=i \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \frac{1}{\delta!} D^{\delta}(\tilde{c}-c)^{\gamma} \times \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} \frac{(g_{00\mu}^p)^{(\delta)}(q')^{a_1}(q'')^{a_2}\ldots(q^{(\gamma)})^{a_\gamma}}{(1!)^{a_1}a_1!(2!)^{a_2}a_2!\ldots(\gamma!)^{a_\gamma}a_\gamma!}, \tag{4.2}$$

$$r_i^q = \gamma_i^q q^{(i)} + Aw_{i-1}^q - \sum_{\mu=1}^{\infty} \sum_{\substack{\delta+\gamma+1=i \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \frac{1}{\delta!} \widetilde{D}^{\delta}(c-\tilde{c})^{\gamma} \times \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} \frac{(g_{00\mu}^q)^{(\delta)}(p')^{a_1}(p'')^{a_2}\ldots(p^{(\gamma)})^{a_\gamma}}{(1!)^{a_1}a_1!(2!)^{a_2}a_2!\ldots(\gamma!)^{a_\gamma}a_\gamma!}, \tag{4.3}$$

$$w_i^p = \sum_{l=1}^{\infty}\sum_{\nu=1}^{l} \frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \sum_{\substack{0\leqslant\delta+\gamma\leqslant i-2l \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} \frac{1}{(1!)^{a_1}a_1!(2!)^{a_2}a_2!\ldots(\gamma!)^{a_\gamma}a_\gamma!} \times \sum_{\substack{\alpha_1+\ldots+\alpha_{l-\nu}+\beta_1+\ldots+\beta_\nu+\delta+\gamma=i \\ \alpha_1,\ldots,\alpha_{l-\nu},\beta_1,\ldots,\beta_\nu\geqslant 2}} \frac{1}{\delta!} D^{\delta}(\widetilde{D}-D)^{\gamma} (g_{l\nu\mu}^p)^{(\delta)}(q')^{a_1}\ldots(q^{(\gamma)})^{a_\gamma} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p r_{\beta_1}^q \ldots r_{\beta_\nu}^q, \tag{4.4}$$

and

$$w_i^q = \sum_{l=1}^{\infty}\sum_{\nu=1}^{l} \frac{(-1)^{l+1}}{l!}\binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \sum_{\substack{0\leqslant\delta+\gamma\leqslant i-2l \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \times \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} \frac{1}{(1!)^{a_1}a_1!(2!)^{a_2}a_2!\ldots(\gamma!)^{a_\gamma}a_\gamma!} \sum_{\substack{\alpha_1+\ldots+\alpha_{l-\nu}+\beta_1+\ldots+\beta_\nu+\delta+\gamma=i \\ \alpha_1,\ldots,\alpha_{l-\nu},\beta_1,\ldots,\beta_\nu\geqslant 2}} \frac{1}{\delta!} \widetilde{D}^{\delta}(D-\widetilde{D})^{\gamma} (g_{l\nu\mu}^q)^{(\delta)}(p')^{a_1}\ldots(p^{(\gamma)})^{a_\gamma} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p r_{\beta_1}^q \ldots r_{\beta_\nu}^q, \tag{4.5}$$

$w_1^p := 0$, $w_1^q := 0$, $i = 2, 3, \ldots, r-1$.

P r o o f. Substituting (3.4), (3.6) and (3.7) into (2.4) and using (4.1) we obtain

$$\begin{aligned}
&s_2^p h^2 + s_3^p h^3 + \ldots + s_i^p h^i + \ldots \\
&\quad = \gamma_2^p h^2 + \gamma_3^p h^3 + \ldots + \gamma_i^p h^i + \ldots + hA(w_2^p h^2 + w_3^p h^3 + \ldots + w_{i-1}^p h^{i-1} + \ldots) \\
&\qquad - hA \sum_{\mu=1}^{\infty} \sum_{i=\mu+1}^{\infty} \sum_{\substack{\delta+\gamma+1=i \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \frac{D^\delta(\tilde{c}-c)^\gamma}{\delta!\gamma!} \\
&\qquad \times \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)'(g_{00\mu}^p)^{(\delta)}(q')^{a_1}(q'')^{a_2}\ldots(q^{(\gamma)})^{a_\gamma} h^i
\end{aligned}$$

and

$$\begin{aligned}
&s_2^q h^2 + s_3^q h^3 + \ldots + s_i^q h^i + \ldots \\
&\quad = \gamma_2^q h^2 + \gamma_3^q h^3 + \ldots + \gamma_i^q h^i + \ldots + h\tilde{A}(w_2^q h^2 + w_3^q h^3 + \ldots + w_{i-1}^q h^{i-1} + \ldots) \\
&\qquad - h\tilde{A} \sum_{\mu=1}^{\infty} \sum_{i=\mu+1}^{\infty} \sum_{\substack{\delta+\gamma+1=i \\ \delta\geqslant 0,\ \gamma\geqslant\mu}} \frac{\widetilde{D}^\delta(c-\tilde{c})^\gamma}{\delta!\gamma!} \\
&\qquad \times \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)'(g_{00\mu}^q)^{(\delta)}(p')^{a_1}(p'')^{a_2}\ldots(p^{(\gamma)})^{a_\gamma} h^i.
\end{aligned}$$

Comparing the terms corresponding to h^i we obtain (4.2) and (4.3).

Substituting (3.6) and (3.7) into (3.1) we have also

$$\begin{aligned}
&w_2^p h^2 + w_3^p h^3 + \ldots + w_i^p h^i + \ldots \\
&= \sum_{l=1}^{\infty} \sum_{\nu=0}^{l} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \frac{1}{\mu!} \big(g_{l\nu\mu}^p I + hD(g_{l\nu\mu}^p)' + \tfrac{1}{2}h^2 D^2 (g_{l\nu\mu}^p)'' + \ldots\big) \\
&\quad \times \mu! \sum_{\gamma=\mu}^{\infty} \frac{(\widetilde{D}-D)^\gamma h^\gamma}{\gamma!} \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)'(q')^{a_1}\ldots(q^{(\gamma)})^{a_\gamma} \\
&\quad \times (r_2^p h^2 + r_3^p h^3 + \ldots)^{l-\nu} (r_2^q h^2 + r_3^q h^3 + \ldots)^\nu \\
&= \sum_{l=1}^{\infty} \sum_{\nu=0}^{l} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \big(g_{l\nu\mu}^p I + hD(g_{l\nu\mu}^p)' + \tfrac{1}{2}h^2 D^2 (g_{l\nu\mu}^p)'' + \ldots\big) \\
&\quad \times \sum_{\gamma=\mu}^{\infty} \frac{(\widetilde{D}-D)^\gamma h^\gamma}{\gamma!} \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)'(q')^{a_1}\ldots(q^{(\gamma)})^{a_\gamma} \\
&\quad \times \sum_{\alpha_1,\ldots,\alpha_{l-\nu}\geqslant 2} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p h^{\alpha_1+\ldots+\alpha_{l-\nu}} \sum_{\beta_1,\ldots,\beta_\nu\geqslant 2} r_{\beta_1}^p \ldots r_{\beta_\nu}^p h^{\beta_1+\ldots+\beta_\nu}
\end{aligned}$$

and

$$
\begin{aligned}
&w_2^q h^2 + w_3^q h^3 + \ldots + w_i^q h^i + \ldots \\
&= \sum_{l=1}^{\infty} \sum_{\nu=0}^{l} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \frac{1}{\mu!} \big(g_{l\nu\mu}^q I + h\widetilde{D}(g_{l\nu\mu}^q)' + \tfrac{1}{2} h^2 \widetilde{D}^2 (g_{l\nu\mu}^q)'' + \ldots \big) \\
&\quad \times \mu! \sum_{\gamma=\mu}^{\infty} \frac{(D-\widetilde{D})^\gamma h^\gamma}{\gamma!} \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)' (p')^{a_1} \ldots (p^{(\gamma)})^{a_\gamma} \\
&\quad \times (r_2^p h^2 + r_3^p h^3 + \ldots)^{l-\nu} (r_2^q h^2 + r_3^q h^3 + \ldots)^\nu \\
&= \sum_{l=1}^{\infty} \sum_{\nu=0}^{l} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \sum_{\mu=0}^{\infty} \big(g_{l\nu\mu}^q I + h\widetilde{D}(g_{l\nu\mu}^q)' + \tfrac{1}{2} h^2 \widetilde{D}^2 (g_{l\nu\mu}^q)'' + \ldots \big) \\
&\quad \times \sum_{\gamma=\mu}^{\infty} \frac{(D-\widetilde{D})^\gamma h^\gamma}{\gamma!} \sum_{\substack{a_1+2a_2+\ldots+\gamma a_\gamma=\gamma \\ a_1+a_2+\ldots+a_\gamma=\mu}} (\gamma; a_1, a_2, \ldots, a_\gamma)' (p')^{a_1} \ldots (p^{(\gamma)})^{a_\gamma} \\
&\quad \times \sum_{\alpha_1,\ldots,\alpha_{l-\nu} \geqslant 2} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p h^{\alpha_1+\ldots+\alpha_{l-\nu}} \sum_{\beta_1,\ldots,\beta_\nu \geqslant 2} r_{\beta_1}^p \ldots r_{\beta_\nu}^p h^{\beta_1+\ldots+\beta_\nu}.
\end{aligned}
$$

Comparing the terms corresponding to h^i we obtain formulas (4.4) and (4.5). □

The relations (4.2), (4.3), (4.4), and (4.5) simplify considerably if $c = \tilde{c}$ (compare also the comment in [7] about the approach based on P-series). In this case these relations assume the form

$$
\begin{aligned}
r_i^p &= \gamma_i^p p^{(i)} + A w_{i-1}^p, \\
r_i^q &= \gamma_i^q q^{(i)} + A w_{i-1}^q, \\
w_i^p &= \sum_{l=1}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\delta=0}^{i-2l} \\
&\qquad \sum_{\substack{\alpha_1+\ldots+\alpha_{l-\nu}+\beta_1+\ldots+\beta_\nu+\delta=i \\ \alpha_1,\ldots,\alpha_{l-\nu},\beta_1,\ldots,\beta_\nu \geqslant 2}} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \frac{D^\delta}{\delta!} (g_{l\nu}^p)^{(\delta)} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p r_{\beta_1}^q \ldots r_{\beta_\nu}^q, \\
w_i^q &= \sum_{l=1}^{\infty} \sum_{\nu=0}^{\infty} \sum_{\delta=0}^{i-2l} \\
&\qquad \sum_{\substack{\alpha_1+\ldots+\alpha_{l-\nu}+\beta_1+\ldots+\beta_\nu+\delta=i \\ \alpha_1,\ldots,\alpha_{l-\nu},\beta_1,\ldots,\beta_\nu \geqslant 2}} \frac{(-1)^{l+1}}{l!} \binom{l}{l-\nu} \frac{D^\delta}{\delta!} (g_{l\nu}^q)^{(\delta)} r_{\alpha_1}^p \ldots r_{\alpha_{l-\nu}}^p r_{\beta_1}^q \ldots r_{\beta_\nu}^q,
\end{aligned}
$$

$w_1^p := 0$, $w_1^q := 0$, $i = 2, 3, \dots, r-1$, where

$$\begin{cases} g_{l\nu}^p(t) := & \dfrac{\partial^l f^p}{\partial p^{l-\nu}\partial q^\nu}\big(t, p(t), q(t)\big), \\ g_{l\nu}^q(t) := & \dfrac{\partial^l f^q}{\partial p^{l-\nu}\partial q^\nu}\big(t, p(t), q(t)\big). \end{cases}$$

5. Computation of order conditions for PRK method of order four

In this section we will illustrate the use of Theorem 4.1 to generate the conditions up to the order four for PRK method (2.1).

Routine calculations lead to

$$\begin{aligned}
r_2^p &= \gamma_2^p p'' - A(\tilde{c}-c)g_{001}^p q', \\
r_2^q &= \gamma_2^q q'' - \tilde{A}(c-\tilde{c})g_{001}^q p', \\
w_2^p &= \gamma_2^p g_{100}^p p'' - A(\tilde{c}-c)g_{100}^p g_{001}^p q' + \gamma_2^q g_{110}^p q'' - \tilde{A}(c-\tilde{c})g_{110}^p g_{001}^q p', \\
w_2^q &= \gamma_2^p g_{100}^q p'' - A(\tilde{c}-c)g_{100}^q g_{001}^p q' + \gamma_2^q g_{110}^q q'' - \tilde{A}(c-\tilde{c})g_{110}^q g_{001}^q p', \\
r_3^p &= \gamma_3^p p^{(3)} - \frac{1}{2}A(\tilde{c}-c)^2 g_{001}^p q'' - AD(\tilde{c}-c)(g_{001}^p)' q' \\
&\quad - \frac{1}{2}A(\tilde{c}-c)^2 g_{002}^p (q')^2 + A\gamma_2^p g_{100}^p p'' - A^2(\tilde{c}-c)g_{100}^p g_{001}^p q' \\
&\quad + A\gamma_2^q g_{110}^p q'' - A\tilde{A}(c-\tilde{c})g_{110}^p g_{001}^q p', \\
r_3^q &= \gamma_3^q q^{(3)} - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{001}^q p'' - \tilde{A}\widetilde{D}(c-\tilde{c})(g_{001}^q)' p' \\
&\quad - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{002}^q (p')^2 + \tilde{A}\gamma_2^p g_{100}^q p'' - \tilde{A}A(\tilde{c}-c)g_{100}^q g_{001}^p q' \\
&\quad + \tilde{A}\gamma_2^q g_{110}^q q'' - \tilde{A}^2(c-\tilde{c})g_{110}^q g_{001}^q p',
\end{aligned}$$

$$\begin{aligned}
w_3^p &= \gamma_3^p g_{100}^p p^{(3)} - \frac{1}{2}A(\tilde{c}-c)^2 g_{100}^p g_{001}^p q'' - AD(\tilde{c}-c)g_{100}^p (g_{001}^p)' q' \\
&\quad - \frac{1}{2}A(\tilde{c}-c)^2 g_{100}^p g_{002}^p (q')^2 + A\gamma_2^p (g_{100}^p)^2 p'' - A^2(\tilde{c}-c)(g_{100}^p)^2 g_{001}^p q' \\
&\quad + A\gamma_2^q g_{100}^p g_{110}^p q'' - A\tilde{A}(c-\tilde{c})g_{100}^p g_{110}^p g_{001}^q p' + D\gamma_2^p (g_{100}^p)' p'' \\
&\quad - DA(\tilde{c}-c)(g_{100}^p)' g_{001}^p q' + (\widetilde{D}-D)\gamma_2^p g_{101}^p q' p'' \\
&\quad - (\widetilde{D}-D)A(\tilde{c}-c)g_{101}^p q' g_{001}^p q' + \gamma_3^q g_{110}^p q^{(3)} - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{110}^p g_{001}^q p'' \\
&\quad - \tilde{A}\widetilde{D}(c-\tilde{c})g_{110}^p (g_{001}^q)' p' - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{110}^p g_{002}^q (p')^2 + \tilde{A}\gamma_2^p g_{110}^p g_{100}^q p'' \\
&\quad - \tilde{A}A(\tilde{c}-c)g_{110}^p g_{100}^q g_{001}^p q' + \tilde{A}\gamma_2^q g_{110}^p g_{110}^q q'' - \tilde{A}^2(c-\tilde{c})g_{110}^p g_{110}^q g_{001}^q p' \\
&\quad + D\gamma_2^q (g_{110}^p)' q'' - D\tilde{A}(c-\tilde{c})(g_{110}^p)' g_{001}^q p' + (\widetilde{D}-D)\gamma_2^q g_{111}^p q' q'' \\
&\quad - (\widetilde{D}-D)\tilde{A}(c-\tilde{c})g_{111}^p q' g_{001}^q p',
\end{aligned}$$

$$
\begin{aligned}
w_3^q = {} & \gamma_3^p g_{100}^q p^{(3)} - \frac{1}{2} A(\tilde{c}-c)^2 g_{100}^q g_{001}^p q'' - AD(\tilde{c}-c) g_{100}^q (g_{001}^p)' q' \\
& - \frac{1}{2} A(\tilde{c}-c)^2 g_{100}^q g_{002}^p (q')^2 + A\gamma_2^p g_{100}^q g_{100}^p p'' - A^2(\tilde{c}-c) g_{100}^q g_{100}^p g_{001}^p q' \\
& + A\gamma_2^q g_{100}^q g_{110}^p q'' - A\tilde{A}(c-\tilde{c}) g_{100}^q g_{110}^p g_{001}^q p' + \widetilde{D}\gamma_2^p (g_{100}^q)' p'' \\
& - \widetilde{D} A(\tilde{c}-c)(g_{100}^q)' g_{001}^p q' + (D-\widetilde{D})\gamma_2^p g_{101}^q p' p'' \\
& - (D-\widetilde{D}) A(\tilde{c}-c) g_{101}^q p' g_{001}^p q' + \gamma_3^q g_{110}^q q^{(3)} - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{110}^q g_{001}^q p'' \\
& - \tilde{A}\widetilde{D}(c-\tilde{c}) g_{110}^q (g_{001}^q)' p' - \frac{1}{2}\tilde{A}(c-\tilde{c})^2 g_{110}^q g_{002}^q (p')^2 + \tilde{A}\gamma_2^p g_{110}^q g_{100}^q p'' \\
& - \tilde{A} A(\tilde{c}-c) g_{110}^q g_{100}^q g_{001}^p q' + \tilde{A}\gamma_2^q (g_{110}^q)^2 q'' - \tilde{A}^2 (c-\tilde{c})(g_{110}^q)^2 g_{001}^q p' \\
& + \widetilde{D}\gamma_2^q (g_{110}^q)' q'' - \widetilde{D}\tilde{A}(c-\tilde{c})(g_{110}^q)' g_{001}^q p' + (D-\widetilde{D})\gamma_2^q g_{111}^q p' q'' \\
& - (D-\widetilde{D})\tilde{A}(c-\tilde{c}) g_{111}^q p' g_{001}^q p'.
\end{aligned}
$$

It follows from Theorem 3.2 that PRK method (2.1) has order four if and only if $\hat{d}_n^p = O(h^r)$, $\hat{d}_n^q = O(h^r)$, $n = 0, 1, \ldots, N$, $b^T w_i^p = O(h^4)$ and $\tilde{b}^T w_i^q = O(h^4)$, $i = 2, 3$. This leads to the following equations expressed only in terms of the coefficients c, A, b, and $\tilde{c}$, $\tilde{A}$, $\tilde{b}$ of PRK method (2.1).

Order 1:	$b^T e = 1,$	$\tilde{b}^T e = 1;$
Order 2:	$b^T c = \frac{1}{2},$	$\tilde{b}^T \tilde{c} = \frac{1}{2},$
	$b^T(\tilde{c}-c) = 0,$	$\tilde{b}^T(c-\tilde{c}) = 0;$
Order 3:	$b^T c^2 = \frac{1}{3},$	$\tilde{b}^T \tilde{c} = \frac{1}{3},$
	$b^T(\tilde{c}-c)^2 = 0,$	$b^T D(\tilde{c}-c) = 0,$
	$\tilde{b}^T(c-\tilde{c})^2 = 0,$	$\tilde{b}^T \tilde{D}(c-\tilde{c}) = 0,$
	$b^T \gamma_2^p = 0,$	$\tilde{b}^T \gamma_2^p = 0,$
	$b^T A(\tilde{c}-c) = 0,$	$\tilde{b}^T A(\tilde{c}-c) = 0,$
	$b^T \gamma_2^q = 0,$	$\tilde{b}^T \gamma_2^q = 0,$
	$b^T \tilde{A}(c-\tilde{c}) = 0,$	$\tilde{b}^T \tilde{A}(c-\tilde{c}) = 0;$
Order 4:	$b^T c^3 = \frac{1}{4},$	$\tilde{b}^T \tilde{c}^3 = \frac{1}{4},$
	$b^T(\tilde{c}-c)^3 = 0,$	$\tilde{b}^T(c-\tilde{c})^3 = 0,$
	$b^T D(\tilde{c}-c)^2 = 0,$	$\tilde{b}^T \widetilde{D}(c-\tilde{c})^2 = 0,$
	$b^T D^2(\tilde{c}-c) = 0,$	$\tilde{b}^T \widetilde{D}^2(c-\tilde{c}) = 0,$
	$b^T \gamma_3^p = 0,$	$\tilde{b}^T \gamma_3^p = 0,$
	$b^T A(\tilde{c}-c)^2 = 0,$	$\tilde{b}^T A(\tilde{c}-c)^2 = 0,$
	$b^T AD(\tilde{c}-c) = 0,$	$\tilde{b}^T AD(\tilde{c}-c) = 0,$
	$b^T A\gamma_2^p = 0,$	$\tilde{b}^T A\gamma_2^p = 0,$
	$b^T A^2(\tilde{c}-c) = 0,$	$\tilde{b}^T A^2(\tilde{c}-c) = 0,$
	$b^T A\gamma_2^q = 0,$	$\tilde{b}^T A\gamma_2^q = 0,$

$$
\begin{array}{ll}
b^T A\tilde{A}(c-\tilde{c}) = 0, & \tilde{b}^T A\tilde{A}(c-\tilde{c}) = 0, \\
b^T D\gamma_2^p = 0, & \tilde{b}^T \widetilde{D}\gamma_2^p = 0, \\
b^T DA(\tilde{c}-c) = 0, & \tilde{b}^T \widetilde{D}A(\tilde{c}-c) = 0, \\
b^T(\widetilde{D}-D)\gamma_2^p = 0, & \tilde{b}^T(D-\widetilde{D})\gamma_2^p = 0, \\
b^T(\widetilde{D}-D)A(\tilde{c}-c) = 0, & \tilde{b}^T(D-\widetilde{D})A(\tilde{c}-c) = 0, \\
b^T\gamma_3^q = 0, & \tilde{b}^T\gamma_3^q = 0, \\
b^T\tilde{A}(c-\tilde{c})^2 = 0, & \tilde{b}^T\tilde{A}(c-\tilde{c})^2 = 0, \\
b^T\tilde{A}\widetilde{D}(c-\tilde{c}) = 0, & \tilde{b}^T\tilde{A}\widetilde{D}(c-\tilde{c}) = 0, \\
b^T\tilde{A}\gamma_2^p = 0, & \tilde{b}^T\tilde{A}\gamma_2^p = 0, \\
b^T\tilde{A}A(\tilde{c}-c) = 0, & \tilde{b}^T\tilde{A}A(\tilde{c}-c) = 0, \\
b^T\tilde{A}\gamma_2^q = 0, & \tilde{b}^T\tilde{A}\gamma_2^q = 0, \\
b^T\tilde{A}^2(c-\tilde{c}) = 0, & \tilde{b}^T\tilde{A}^2(c-\tilde{c}) = 0, \\
b^T D\gamma_2^q = 0, & \tilde{b}^T\widetilde{D}\gamma_2^q = 0, \\
b^T D\tilde{A}(c-\tilde{c}) = 0, & \tilde{b}^T\widetilde{D}\tilde{A}(c-\tilde{c}) = 0, \\
b^T(\widetilde{D}-D)\gamma_2^q = 0, & \tilde{b}^T(D-\widetilde{D})\gamma_2^q = 0, \\
b^T(\widetilde{D}-D)\tilde{A}(c-\tilde{c}) = 0, & \tilde{b}^T(D-\widetilde{D})\tilde{A}(c-\tilde{c}) = 0.
\end{array}
$$

In the case $c = \tilde{c}$ these conditions reduce to the following much smaller set of equations listed below.

$$
\begin{array}{lll}
\text{Order 1:} & b^T e = 1, & \tilde{b}^T e = 1; \\
\text{Order 2:} & b^T c = \frac{1}{2}, & \tilde{b}^T c = \frac{1}{2}; \\
\text{Order 3:} & b^T c^2 = \frac{1}{3}, & \tilde{b}^T c = \frac{1}{3}, \\
 & b^T\gamma_2^p = 0, & \tilde{b}^T\gamma_2^p = 0, \\
 & b^T\gamma_2^q = 0, & \tilde{b}^T\gamma_2^q = 0; \\
\text{Order 4:} & b^T c^3 = \frac{1}{4}, & \tilde{b}^T c^3 = \frac{1}{4}, \\
 & b^T\gamma_3^p = 0, & \tilde{b}^T\gamma_3^p = 0, \\
 & b^T A\gamma_2^p = 0, & \tilde{b}^T A\gamma_2^p = 0, \\
 & b^T A\gamma_2^q = 0, & \tilde{b}^T A\gamma_2^q = 0, \\
 & b^T D\gamma_2^p = 0, & \tilde{b}^T D\gamma_2^p = 0, \\
 & b^T\gamma_3^q = 0, & \tilde{b}^T\gamma_3^q = 0, \\
 & b^T\tilde{A}\gamma_2^p = 0, & \tilde{b}^T\tilde{A}\gamma_2^p = 0, \\
 & b^T\tilde{A}\gamma_2^q = 0, & \tilde{b}^T\tilde{A}\gamma_2^q = 0, \\
 & b^T D\gamma_2^q = 0, & \tilde{b}^T D\gamma_2^q = 0.
\end{array}
$$

These relations are equivalent to the order conditions listed in [5].

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References

[1] *M. Abramowitz, I. S. Stegun (eds.)*: Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. National Bureau of Standards, Applied Mathematics Series 55, Washington, D.C., 1972.

[2] *P. Albrecht*: A new theoretical approach to Runge-Kutta methods. SIAM J. Numer. Anal. *24* (1987), 391–406.

[3] *P. Albrecht*: The Runge-Kutta theory in a nutshell. SIAM J. Numer. Anal. *33* (1996), 1712–1735.

[4] *H. Brunner, E. Hairer and S. P. Nørsett*: Runge-Kutta theory for Volterra integral equations of the second kind. Math. Comp. *39* (1982), 147–163.

[5] *E. Griepentrog*: Gemischte Runge-Kutta-Verfahren für steife Systeme. In: Seminarbericht Nr. 11, Sekt. Math., Humboldt Univ. Berlin, 1978, pp. 19–29.

[6] *E. Hairer*: Order conditions for numerical methods for partitioned ordinary differential equations. Numer. Math. *36* (1981), 431–445.

[7] *E. Hairer, S. P. Nørsett and G. Wanner*: Solving Ordinary Differential Equations I. Nonstiff Problems. Springer-Verlag, Berlin-Heidelberg-New York, 1991.

[8] *Z. Jackiewicz, R. Vermiglio*: General linear methods with external stages of different orders. BIT *36* (1996), 688–712.

[9] *Z. Jackiewicz, S. Tracogna*: A general class of two-step Runge-Kutta methods for ordinary differential equations. SIAM J. Numer. Anal. *32* (1995), 1390–1427.

[10] *Z. Jackiewicz, S. Tracogna*: Variable stepsize continuous two-step Runge-Kutta methods for ordinary differential equations. Numer. Algorithms *12* (1996), 347–368.

[11] *J. M. Sanz-Serna, M. P. Calvo*: Numerical Hamiltonian Problems. Chapman & Hall, London-Glasgow-New York, 1994.

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