Implicit Runge-Kutta schemes for optimal control problems with evolution equations

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Abstract

In this paper we discuss the use of implicit Runge-Kutta schemes for the time discretization of optimal control problems with evolution equations. The specialty of the considered discretizations is that the discretizations schemes for the state and adjoint state are chosen such that discretization and optimization commute. It is well known that for Runge-Kutta schemes with this property additional order conditions are necessary. We give sufficient conditions for which class of schemes these additional order condition are automatically fulfilled. The focus is especially on implicit Runge-Kutta schemes of Gauss, Radau IA, Radau IIA, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC collocation type up to order six. Furthermore we also use a SDIRK (singly diagonally implicit Runge-Kutta) method to demonstrate, that for general implicit Runge-Kutta methods the additional order conditions are not automatically fulfilled.

Numerical examples illustrate the predicted convergence rates.

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1. Introduction

The novelty of this contribution is the characterization for which implicit Runge-Kutta schemes for distributed parabolic optimal control problems discretization and optimization commute and the convergence order is preserved. This characterization is done in terms of simplifying assumptions for the coefficients of the schemes. The commutability is desired for the following reasons. For the approach discretize-then-optimize we can choose an appropriate approximations for the state and the adjoint equation but we might need to transfer discrete quantities from one discretization to the other discretization. This may result in an solution operator which is not symmetric and positive definite. On the other hand if we chose the other approach optimize-then-discretize we do not have this problem, but we also do not know if the discrete adjoint state is an appropriate approximation of the continuous adjoint state. Therefore our goal is to use schemes which combine the advantages of both approaches.

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In particular we discuss higher order time discretization with implicit Runge-Kutta schemes for the optimal control problem

\[
\begin{aligned}
\min & \frac{1}{2} \left\| M^{1/2} (y(\cdot, T) - y_D) \right\|_H^2 + \int_0^T \nu \frac{1}{2} \left\| M^{1/2} u \right\|_H^2 \, dt,
\end{aligned}
\]

\[
\begin{align*}
M y_t + A y &= B u, \\
M y(0) &= M v,
\end{align*}
\]

with the control \( u \) and the state \( y \). The Hilbert space \( H \) is appropriately chosen, the desired state \( y_D \in H \) and the initial condition \( v \in H \) are given, and the operators \( M \) and \( B \) are regular. Further we assume that the operator \( A \) is self-adjoint, and maps \( A : V \rightarrow V^* \) with the Hilbert space \( V \subseteq H \). In the case of second order parabolic equations we choose \( H^1(\Omega) \subseteq V \subseteq H^1_0(\Omega) \), corresponding to the boundary conditions, and \( H = L^2(\Omega) \).

Due to the papers of Becker, Meidner and Vexler [2] and Meidner and Vexler [18, 19] it is well known that discretization and optimization commute for continuous and discontinuous Galerkin time discretizations. The work on discontinuous Galerkin schemes [18] provides error estimates for time discretization of arbitrary order, whereas the continuous Galerkin case was limited to the Petrov-Galerkin Crank-Nicolson scheme [19].

Lasaint and Raviart [16] have proven the equivalence of discontinuous Galerkin time discretization to special implicit Runge-Kutta schemes. But there are also time stepping schemes, for which the equivalence to Galerkin schemes is not clear and for which discretization and optimization commute. A second order time stepping Crank-Nicolson scheme, for which discretization and optimization commute and which is not a Galerkin scheme, is discussed, among other variants, in a paper by Apel and Flaig [1]. Previous papers on Crank-Nicolson time discretizations, as Rösch [20], did not provide results on second order convergence.

For the time discretization of optimal control problems it is well known, that Runge-Kutta schemes which provide the commutation of discretization and optimization need to fulfill additional order conditions, see Hager [7, 8] and Bonnans and Laurent-Varin [3, 4]. In [3, 4] no numerical discretization schemes, which fulfill these conditions, were given and in [8] only numerical examples with explicit Runge-Kutta schemes were presented. The analysis was extended to W-method by Lang and Verwer and the additional order conditions up to order three can be found in [15]. Herty, Pareschi and Steffensen [12, 13] transfer the theory of Hager and Bonnans and Laurent-Varin to implicit-explicit discretizations, where the stiff part of the differential equation is discretized with an implicit scheme and the non-stiff part with an explicit scheme. They give order conditions up to order three.

In this contribution we focus on \( A \)-stable discretization schemes for the discretization of a parabolic equation and therefore on implicit Runge-Kutta schemes. For schemes up to order six we give simple criteria for the decision whether the additional order conditions are fulfilled. These criteria are given in terms of well known simplifying assumptions on the coefficients of Runge-Kutta schemes. In particular we see that collocation Runge-Kutta schemes of Gauss, Radau IA, Radau IIA, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC type fulfill the additional order conditions. We also give an SDIRK scheme as example for which the additional conditions do not hold and the order reduction can be observed.

The outline of the paper is as follows. In the next section we introduce the time discretization and in Section 3 we analyze under which circumstances the additional order conditions are fulfilled. In Section 4 numerical examples confirm the predicted orders of convergence.
2. Time Discretizations

2.1. Runge-Kutta schemes for the time discretization of optimal control problems

It is well known \[17, 21\] that the first order optimality conditions for the optimal control problem \((1)\) are given by

\[
\begin{align*}
M \ddot{y} + A \dot{y} &= B \ddot{u}, \\
M \dot{y}(0) &= M \ddot{v}, \\
M \ddot{p} - A \dot{p} &= 0, \\
M \dot{p}(T) &= M (y_D - \ddot{y}(T)), \\
M \ddot{u} &= \frac{1}{\nu} M \ddot{p}.
\end{align*}
\]

(2)

Since the problem \((1)\) is convex these necessary optimality conditions are also sufficient. As seen in \[4, Formula (6)\] and \[7, 8\] for the \(s\)-stage Runge-Kutta discretization of the optimal control problem \((1)\) given by

\[
\begin{align*}
M \ddot{y}_{k+1} &= M \ddot{y}_k + \tau_k \sum_{i=1}^{s} b_i (M \ddot{u}_{k;i} - A \ddot{y}_{k;i}), \\
M \ddot{y}_{k;i} &= M \ddot{y}_k + \tau_k \sum_{j=1}^{s} a_{ij} (M \ddot{u}_{k;j} - A \ddot{y}_{k;j}), \\
M \ddot{p}_{k+1} &= M \ddot{p}_k - \tau_k \sum_{i=1}^{s} \hat{b}_i A \ddot{p}_{k;i}, \\
M \ddot{p}_{k;i} &= M \ddot{p}_k - \tau_k \sum_{j=1}^{s} \hat{a}_{ij} A \ddot{p}_{k;j}, \\
M \ddot{u}_{k;i} &= \frac{1}{\nu} M \ddot{p}_{k;i}, \\
M \ddot{y}_0 &= M \ddot{v}, \\
M \ddot{p}_N &= M (y_D - \ddot{y}_N),
\end{align*}
\]

(3)

discretization and optimization commute if the two schemes for the state and the adjoint state fulfill the conditions

\[
\begin{align*}
\hat{b}_i &= b_i, \\
\hat{a}_{ij} &= b_j - b_i \frac{a_{ji}}{b_i}.
\end{align*}
\]

(4)

In the discretization \((3)\) we denote the discretization of the state and the adjoint state for \(t = t_k\) by \(\ddot{y}_k, \ddot{p}_k\), the inner stages of the Runge-Kutta schemes by \(\ddot{y}_{k;i}, \ddot{p}_{k;i}\) and the time step size by \(\tau_k\).

The conditions \((4)\) are also known as condition for symplecticity of partitioned Runge-Kutta schemes \[9, Theorem VI.4.6\].

For the Runge-Kutta discretization of optimal control problems it is known (see \[8, 4, 8\]) that in addition to the usual order conditions additional order conditions are needed. These conditions were given in \[8, Table 1\] up to order four and in \[4, Table 2–6\] up to order six. We repeat these order conditions up to order four in Table \[1\] the conditions of order five in Table \[2\] and the conditions of order six in the Tables \[3, 4\].
Table 1: The order conditions for Runge-Kutta discretization for the state equation and optimal control problems, see also [4, Table 2–4][8, Table 1 and 2]. All summations go from 1 to the number of stages $s$.

(a) Abbreviations

$$c_i = \sum a_{ij}, \quad d_j = \sum b_i a_{ij}.$$ 

(b) Order conditions for the state equation without control

| Order | Conditions                                      | (O1)  | (O2)  | (O3)  | (O4)  |
|-------|------------------------------------------------|-------|-------|-------|-------|
| 1     | $\sum b_i = 1.$                                 |       |       |       |       |
| 2     | $\sum d_i = \frac{1}{2}.$                       |       |       |       |       |
| 3     | $\sum c_i d_i = \frac{1}{6}, \quad \sum b_i c_i^2 = \frac{1}{3}$ |       |       |       |       |
| 4     | $\sum b_i c_i^3 = \frac{1}{4}, \quad \sum b_i c_i a_{ij} = \frac{1}{5}, \quad \sum d_i c_i^2 = \frac{1}{12}, \quad \sum d_i a_{ij} c_j = \frac{1}{24}.$ |       |       |       |       |

(c) Additional order conditions for optimal control problems

| Order | Additional conditions                          | (A3)  | (A4)  |
|-------|------------------------------------------------|-------|-------|
| 3     | $\sum \frac{d_i^2}{b_i} = \frac{1}{3}.$      |       |       |
| 4     | $\sum \frac{c_i d_i^2}{b_i} = \frac{1}{12}, \quad \sum \frac{d_j^3}{b_j^2} = \frac{1}{4}, \quad \sum \frac{b_j c_i a_{ij} d_j}{b_j} = \frac{5}{24}, \quad \sum \frac{d_i a_{ij} d_j}{b_j} = \frac{1}{8}.$ |       |       |
Table 2: The order conditions of order 5 for Runge-Kutta discretization for the state equation and optimal control problems, see also [4, Table 6]. All summations go from 1 to the number of stages $s$.

(a) Order conditions of order 5 for the state equation without control (computed with Mathematica).

\[
\begin{align*}
\sum b_i a_{ik} a_{kj} c_i c_j &= \frac{1}{30}, \\
\sum a_{jk} c_j d_j c_k &= \frac{1}{40}, \\
\sum b_i a_{ij} c_i c_j^2 &= \frac{1}{15}, \quad (O5-1) \\
\sum c_i^3 d_j &= \frac{1}{20}, \\
\sum b_i a_k a_{il} c_i d_k &= \frac{11}{120}, \\
\sum b_i a_{ij} c_i^2 c_j &= \frac{1}{10}, \quad (O5-2) \\
\sum a_{kj} c_j^2 d_k &= \frac{1}{60}, \\
\sum b_i c_i^4 &= \frac{1}{5}, \\
\sum b_i \left( \sum a_{ij} c_j \right)^2 &= \frac{1}{20}, \quad (O5-3)
\end{align*}
\]

(b) Additional order conditions of order 5 for optimal control problems (see also [4, Table 6]).

\[
\begin{align*}
\sum \frac{1}{b_k} a_{ik} c_k d_k d_l &= \frac{1}{40}, \\
\sum \frac{1}{b_k} a_{ik}^2 c_k^2 d_l &= \frac{1}{30}, \\
\sum \frac{1}{b_l} c_l d_l^3 &= \frac{1}{20}, \quad (A5-1) \\
\sum \frac{1}{b_k} a_{kl} d_k^2 c_l &= \frac{1}{60}, \\
\sum \frac{1}{b_m} d_m^4 &= \frac{1}{5}, \\
\sum b_{lk} a_{ik} c_i c_j &= \frac{1}{20}, \quad (A5-2) \\
\sum a_{lk} a_{kj} c_l d_l &= \frac{1}{120}, \\
\sum \frac{1}{b_k} a_{lk} d_k c_l d_l &= \frac{7}{120}, \\
\sum b_{lk} a_{jk} c_i c_j &= \frac{2}{15}, \quad (A5-3) \\
\sum b_{lk} a_{ik} c_i c_k d_k &= \frac{7}{120}, \\
\sum b_{lk} a_{il} d_i c_i d_i &= \frac{3}{20}, \\
\sum \frac{1}{b_k} a_{mk} a_{ik} d_i d_m &= \frac{1}{20}, \quad (A5-4) \\
\sum \frac{1}{b_l} a_{ml} d_l^2 d_m &= \frac{1}{10}, \\
\sum \frac{1}{b_k} a_{ml} a_{lk} d_k d_m &= \frac{1}{30}, \\
\sum \frac{1}{b_k} a_{lk} a_{ik} c_i d_l &= \frac{3}{40}, \quad (A5-5) \\
\sum \frac{1}{b_k} a_{ik} a_{il} d_i c_l &= \frac{3}{40}, \\
\sum \frac{b_l}{b_i} a_{im} a_{il} d_m d_m &= \frac{2}{15}, \\
\sum \frac{b_l}{b_k} a_{ik} c_i^2 d_k &= \frac{3}{20}, \quad (A5-6) \\
\sum \frac{1}{b_l b_m} a_{lm} d_l^2 d_m &= \frac{1}{15}. \quad (A5-7)
\end{align*}
\]
Table 3: The order conditions of order 6 for Runge-Kutta discretization for the state equation without control (computed with Mathematica). All summations go from 1 to the number of stages \( s \).

\[
\begin{align*}
\sum c_i^4 d_j \ &= \frac{1}{30}, \\
\sum a_{lm} a_{lk} a_{jk} d_j c_m \ &= \frac{1}{720}, \\
\sum b_i a_{ij} c_i^2 c_j^2 \ &= \frac{1}{18}, \quad (O6-1) \\
\sum a_{jk} c_j d_j c_k^2 \ &= \frac{1}{90}, \\
\sum b_i a_{ij} c_i^3 c_j \ &= \frac{1}{24}, \\
\sum a_{k j} c_j^3 d_k \ &= \frac{1}{120}, \quad (O6-2) \\
\sum b_i a_{ij} c_i^4 c_j \ &= \frac{1}{12}, \\
\sum a_{jk} c_j^2 d_j c_k \ &= \frac{1}{60}, \\
\sum b_i a_{ij} a_{jk} c_j c_k \ &= \frac{1}{48}, \quad (O6-3) \\
\sum a_{ij} a_{jk} c_j c_k d_i \ &= \frac{1}{240}, \\
\sum a_{ik} a_{ij} c_j c_i \ &= \frac{1}{180}, \\
\sum b_i a_{ij} a_{ij} c_i^2 c_j \ &= \frac{1}{36}, \quad (O6-4) \\
\sum b_i a_{ik} a_{ij} c_j c_i d_i \ &= \frac{1}{72}, \\
\sum a_{ik} a_{ij} a_{ij} c_i c_j \ &= \frac{1}{144}, \\
\sum b_i c_i^5 \ &= \frac{1}{6}, \quad (O6-5) \\
\sum b_i c_i (\sum a_{ij} c_j) ^2 \ &= \frac{1}{24}, \\
\sum b_i a_{ij} (\sum a_{jk} c_k) ^2 \ &= \frac{1}{120}. \quad (O6-7)
\end{align*}
\]

Table 4: Part 1 of the additional order conditions of order 6 for Runge-Kutta discretization for optimal control problems, see also [4] Table 6]. All summations go from 1 to the number of stages \( s \).

\[
\begin{align*}
\sum \frac{1}{b_k} d_i^6 \ &= \frac{1}{6}, \\
\sum \frac{1}{b_k} c_i^m d_i^4 \ &= \frac{1}{30}, \\
\sum \frac{1}{b_k} c_i^2 d_i^4 \ &= \frac{1}{60}, \quad (A6-1) \\
\sum \frac{1}{b_k} c_i^2 c_k^2 d_i \ &= \frac{1}{60}, \\
\sum b_i a_{ik} c_i^2 c_k d_k \ &= \frac{2}{45}, \\
\sum \frac{1}{b_k} a_{jk} c_j c_k d_i \ &= \frac{7}{60}, \quad (A6-2) \\
\sum b_i b_k c_i^2 c_k^2 \ &= \frac{1}{180}, \\
\sum b_i b_k a_{ik} c_i^2 c_k d_k \ &= \frac{2}{45}, \\
\sum \frac{1}{b_k} a_{jm} d_i^2 c_m d_m \ &= \frac{2}{45}, \\
\sum \frac{1}{b_k} b_k b_m a_{jm} d_i^2 d_m \ &= \frac{1}{18}, \quad (A6-3) \\
\sum \frac{1}{b_k} a_{kl} d_i^2 c_k^2 \ &= \frac{1}{180}, \\
\sum \frac{1}{b_k} a_{kl} d_i^2 c_k d_k \ &= \frac{1}{90}, \\
\sum \frac{1}{b_k} b_k a_{ik} c_i^2 c_k d_k \ &= \frac{7}{60}, \quad (A6-4) \\
\sum b_i b_k a_{ik} c_i^2 c_k d_k \ &= \frac{1}{40}, \\
\sum \frac{1}{b_k} a_{ik} d_i^2 c_k d_k \ &= \frac{1}{120}, \\
\sum \frac{1}{b_k} a_{ik} c_i^2 c_k d_k \ &= \frac{1}{30}, \quad (A6-5) \\
\sum b_i b_k a_{ik} c_i^2 c_k d_k \ &= \frac{1}{40}, \\
\sum \frac{1}{b_k} a_{ik} d_i^2 c_k^2 \ &= \frac{1}{60}, \\
\sum \frac{1}{b_k} a_{ik} d_i^2 c_k d_k \ &= \frac{1}{120}, \quad (A6-6) \\
\sum \frac{1}{b_k} a_{im} c_i^3 d_m \ &= \frac{7}{60}, \\
\sum \frac{1}{b_k} a_{im} c_i^3 d_m \ &= \frac{1}{12}. \quad (A6-7)
\end{align*}
\]
Table 5: Part 2 of the additional order conditions of order 6 for Runge-Kutta discretization for optimal control problems, see also [4] Table 6. All summations go from 1 to the number of stages $s$.

\[
\begin{align*}
\sum \frac{a_{im}d^3c_m}{b_i^3} & = \frac{1}{120}, \\
\sum \frac{a_{nn}d^3d_m}{b_n^2b_m} & = \frac{1}{24}, \\
\sum \frac{a_{mk}a_{lk}c_kd_m}{b_k} & = \frac{1}{120} \quad (A6-8) \\
\sum \frac{a_{mn}a_{il}d^2d_m}{b_n b_m} & = \frac{1}{48}, \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{11}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-9) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-10) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-11) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-12) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-13) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-14) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-15) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-16) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-17) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-18) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-19) \\
\sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} & = \frac{7}{120}, \quad \sum \frac{b_{i}a_{im}a_{il}c_jd_m}{b_k} = \frac{1}{24} \quad (A6-20)
\end{align*}
\]
Table 6: Part 3 of the additional order conditions of order 6 for Runge-Kutta discretization for optimal control problems, see also [4, Table 6]. All summations go from 1 to the number of stages $s$.

\[
\sum b_j a_j a_k c_j c_j = \frac{1}{18}, \quad \sum b_i b_j a_j a_k c_i c_l = \frac{7}{144}, \quad (A6-21)
\]
\[
\sum b_i b_j a_j a_k c_i c_l = \frac{61}{720}, \quad \sum b_i a_i a_i a_k d_i c_i = \frac{7}{360}, \quad (A6-22)
\]
\[
\sum b_i a_i a_i c_i c_k = \frac{19}{720}, \quad \sum b_i a_i a_i a_k d_i c_i = \frac{13}{360}, \quad (A6-23)
\]
\[
\sum a_n a_m a_n d_i d_i = \frac{1}{18}, \quad \sum b_i a_i a_i a_k d_i c_i = \frac{7}{360}, \quad (A6-24)
\]
\[
\sum a_m a_m a_n d_i d_i = \frac{1}{144}, \quad \sum b_i a_i a_i a_k d_i c_i = \frac{13}{360}, \quad (A6-25)
\]
\[
\sum a_n a_m a_i d_i d_i = \frac{1}{72}, \quad \sum b_i a_i a_i a_k d_i c_i = \frac{19}{720}, \quad (A6-26)
\]
\[
\sum b_i a_i a_i a_i d_i d_i = \frac{7}{144}, \quad (A6-27)
\]

2.2. Implicit Runge-Kutta discretizations for optimal control problems

For our discussion we focus on implicit collocation Runge-Kutta schemes of of Gauss, Radau IA, Radau IIA, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC type up to order 6 and a SDIRK method of order four. The corresponding Butcher tableaux are repeated in Table 7–10. In the selection of schemes the focus was on $A$-stable Runge-Kutta schemes of higher order. Additionally the Störmer Verlet scheme of order two was included, as this gives a new variant of the results of [1, 6]. Whereas in [1, 6] the state and the adjoint state were discretized on shifted time meshes, in the discretization (3) the state and the adjoint state are discretized on the same time mesh. The corresponding discretization schemes for the adjoint equation are given by the relation (4).

Remark 2.1. In some cases the adjoint schemes of the Runge-Kutta discretizations are well known schemes of their own:

- The scheme for the adjoint discretization of the Gauss scheme is the Gauss scheme itself.
- The scheme for the adjoint discretization of the Lobatto IIIA scheme is the Lobatto IIIB scheme and vice versa (see also [9]).
- The scheme for the fourth order adjoint discretization of the Lobatto IIIC scheme is known as Butcher’s Lobatto scheme. This scheme is not $A$-stable (see [11, Example IV.3.5.]).
- The scheme for the adjoint discretization of the Radau IA scheme is known not to be $A$-stable (see [11, Example IV.3.5.]).
Table 7: Coefficients of Runge Kutta schemes of order two and three (see also [9, 10, 11]).

(a) Coefficients of the Störmer-Verlet discretization for the state (cf. [9, Table 2.1]).

(b) Coefficients for the Radau IA method of order three (cf. [11, Table IV.5.3.]).

(c) Coefficients for the Radau IIA method of order three (cf. [11, Table IV.5.5.]).

Table 8: Coefficients of Runge Kutta schemes of order four (see also [9, 10, 11]).

(a) Coefficients for the Gauss scheme of order four (cf. [10, Table II.7.3], [11, Table IV.5.1.]).

(b) Coefficients for an $L$-stable SDIRK method of order four (cf. [11, Formula (6.16)]).

(c) Coefficients for the Lobatto IIIA method of order four (cf. [11, Table IV.5.7.]).

(d) Coefficients for the Lobatto IIB method of order four (cf. [11, Table IV.5.9.]).

(e) Coefficients for the Lobatto IIC method of order four (cf. [11, Table IV.5.11.]).
Table 9: Coefficients of Runge Kutta schemes of order five (see also [9, 10, 11]).

(a) Coefficients for the Radau I A method of order five (cf. [11, Table IV.5.3]).

|   | 0 | $-1 - \sqrt{5}$ | $-1 + \sqrt{5}$ | $4 - \sqrt{6}$ | $88 - 7\sqrt{6}$ | $296 - 169\sqrt{6}$ | $-2 + 3\sqrt{5}$ |
|---|---|-----------------|-----------------|-----------------|-------------------|---------------------|------------------|
|   | 0 | $\frac{1}{9}$   | $\frac{1}{18}$  | $\frac{1}{18}$  | $\frac{10}{360}$  | $\frac{1800}{1800}$  | $\frac{225}{225}$ |
| $6 - \sqrt{5}$ | $\frac{1}{9}$ | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  |
| $6 + \sqrt{5}$ | $\frac{1}{9}$ | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  | $\frac{1}{36}$  |

(b) Coefficients for the Radau IIA method of order five (cf. [11, Table IV.5.5]).

|   | 1 | $16 - \sqrt{5}$ | $16 + \sqrt{5}$ |
|---|---|-----------------|-----------------|
|   | 1 | $\frac{1}{36}$  | $\frac{1}{36}$  |

Table 10: Coefficients of Runge Kutta schemes of order six (see also [9, 10, 11]).

(a) Coefficients for the Gauss scheme of order six (cf. [11, Table IV.5.2]).

|   | $\frac{1}{2} - \frac{\sqrt{15}}{10}$ | $\frac{5}{36}$ | $\frac{2}{9} - \frac{\sqrt{15}}{15}$ | $\frac{5}{36} - \frac{\sqrt{15}}{30}$ |
|---|-----------------------------------|----------------|-----------------------------------|-----------------------------------|
|   | $\frac{1}{2} + \frac{\sqrt{15}}{10}$ | $\frac{5}{36}$ | $\frac{2}{9} + \frac{\sqrt{15}}{15}$ | $\frac{5}{36}$ |
|   | $\frac{1}{12}$ | $\sqrt{5}$ | $\frac{5}{12}$ | $\frac{1}{12}$ |
|   | $\frac{1}{12}$ | $\sqrt{5}$ | $\frac{5}{12}$ | $\frac{1}{12}$ |

(b) Coefficients for the Lobatto IIIC method of order six (cf. [11, Table IV.5.11]).

(c) Coefficients for the Lobatto IIIA method of order six (cf. [11, Table IV.5.7]).

(d) Coefficients for the Lobatto IIIB method of order six (cf. [11, Table IV.5.9]).
Next we investigate the convergence of implicit Runge-Kutta schemes for optimal control problems.

3. Convergence order of the Runge-Kutta discretizations

For the convergence of the Runge-Kutta discretization of the optimal control problem, one could check the order conditions. But we want to further classify the schemes, for which the order conditions for optimal control problems hold. Therefore we recall the simplifying assumptions on the coefficients of a Runge-Kutta scheme. These conditions were introduced for the construction of implicit Runge-Kutta schemes.

**Assumption 3.1 (Simplifying assumptions).** [11, Chapter IV.5] The simplifying assumptions are given by

\[ \sum_{i=1}^{s} b_i c_i^{q-1} = \frac{1}{q}, \quad \text{for } q = 1, \ldots, p, \quad (B(p)) \]

\[ \sum_{j=1}^{s} a_{ij} c_j^{q-1} = \frac{c_j^q}{q}, \quad \text{for } i = 1, \ldots, s, \ q = 1, \ldots, \eta, \quad (C(\eta)) \]

\[ \sum_{i=1}^{s} b_i c_i^{q-1} a_{ij} = \frac{b_j}{q} \left( 1 - c_j^q \right), \quad \text{for } j = 1, \ldots, s, \ q = 1, \ldots, \zeta. \quad (D(\zeta)) \]

Note that the condition \((D(\zeta))\) for \(\zeta = 1\) is equivalent to

\[ d_j = \sum_{i=1}^{s} b_i a_{ij} = b_j (1 - c_j), \]

which will be often used in the proofs later on. So we can characterize easily the order four schemes, which fulfill the additional order conditions automatically.

**Theorem 3.2.** Every third or fourth order Runge-Kutta scheme, for which the simplifying assumption \((D(\zeta))\) for \(\zeta = 1\) holds, fulfills the additional order conditions of order three or four respectively.

**Proof.** This proof can be done with the same ideas as the proof of [8, Proposition 6.1] for explicit Runge-Kutta schemes. With the condition \((D(\zeta))\) for \(\zeta = 1\) the additional conditions of order three and four follow directly of the order conditions from the implicit Runge-Kutta scheme, see [8, Proposition 6.1].

**Corollary 3.3.** The Störmer-Verlet scheme applied to an optimal control problem gives a second order approximation, the application of the two stage Radau IA and Radau IIA schemes gives approximation of order three and the application of the two stage Gauss and the three stage Lobatto IIIA, Lobatto IIIB or Lobatto IIIC schemes gives approximations of order four.

**Proof.** As the scheme of Tables [7a] is only of second order, no further conditions must be fulfilled. As seen in [11, Table IV.5.13] the simplifying assumptions holds for the discussed collocation methods, so this corollary follows directly of the Theorem 3.2.

Next we discuss the convergence of the remaining fourth order scheme.
Theorem 3.4. The pairing of the fourth order SDIRK scheme of Table 8 with the corresponding adjoint scheme applied to an optimal control problem provides only a second order approximation.

Proof. It is well known that the SDIRK scheme of Table 8 is a fourth order scheme, see [11, Table IV.6.5]. For the falsification of the additional order conditions of order three we see that

$$\sum_{i=1}^{s} \frac{d_i^2}{b_i} = \frac{18367}{58800} \neq \frac{1}{3},$$

and therefore the application to optimal control problem is only of order two, as for order two no additional order conditions are needed.

Remark 3.5. It is easy to check that the schemes of Table 8 and the corresponding adjoint scheme are both of order four. Nevertheless the pairing applied to optimal control problems is only of order two, so we see that the conditions in Table 1c are really additional conditions and are not automatically fulfilled for any implicit Runge-Kutta scheme of the corresponding order for ordinary differential equations.

Remark 3.6. The result of Theorem 3.4 is not a general property of SDIRK schemes. There are also SDIRK schemes for which in the discretization (3), (4) the convergence order is preserved, e.g. the SDIRK methods denoted to Crouzeix and Raviart in [11, Exercise IV.6.1], [10, Table II.7.2] of order four with three stages and order three with two stages.

After the classification of fourth order Runge-Kutta schemes for optimal control, we now consider fifth order schemes.

Theorem 3.7. If a Runge-Kutta scheme of order five fulfills the simplifying assumptions (B(p)), (C(\eta)), (D(\zeta)) up to \(p = 2, \eta = 2, \zeta = 2\), then the additional order conditions are also fulfilled.

Proof. The full proof is given in the Appendix A and done by algebraic manipulation of the additional order condition with the simplifying assumptions and the usual order conditions.

Corollary 3.8. The three stage Radau IA and Radau IIA implicit Runge-Kutta schemes applied to an optimal control problem are of order five.

Proof. As seen in [11, Table IV.5.13] the schemes fulfill at least the simplifying assumptions (B(p)), (C(\eta)), (D(\zeta)) up to \(p = 2, \eta = 2, \zeta = 2\).

Theorem 3.9. If a Runge-Kutta scheme of order six fulfills the simplifying assumptions (B(p)), (C(\eta)), (D(\zeta)) up to \(p = 4, \eta = 2, \zeta = 2\), then the additional order conditions are also fulfilled.

Proof. The full proof was carried out by hand by the author by algebraic manipulation of the additional order condition with the simplifying assumptions and the usual order conditions. As this tedious proof gives no higher insights and is, due to the huge number of order conditions, longer as the proof of Theorem 3.7 the details are omitted.

Corollary 3.10. The three stage Gauss and the four stage Lobatto IIIA, Lobatto IIIB and Lobatto IIIC implicit Runge-Kutta schemes applied to an optimal control problem are of order six.
Proof. As seen in [11, Table IV.5.13] the schemes fulfill at least the simplifying assumptions \( B(p) \), \( C(\eta) \), \( D(\zeta) \) up to \( p = 4, \eta = 2, \zeta = 2 \). □

With Theorem 3.2, Theorem 3.7 and Theorem 3.9 we have sufficient conditions if the additional order conditions are fulfilled which are easy to check. It is open whether these conditions are also necessary or if there exists an implicit Runge-Kutta scheme which fulfills the additional order conditions but not the simplifying assumptions.

**Remark 3.11** (Full discretization). In this section the focus was on the time discretization error. The full discretization of a parabolic optimal control problem can be handled with the method of lines as in [11]. Then the error can be split into

\[
\| \tilde{y}(\cdot, t_i) - \bar{y}_h \|_{L^2(\Omega)} + \| \tilde{p}(\cdot, t_i) - \bar{p}_h \|_{L^2(\Omega)} \lesssim \| \tilde{y}(\cdot, t_i) - y_h(t_i) \|_{L^2(\Omega)} + \| y_h(t_i) - \bar{y}_h \|_{L^2(\Omega)} \\
+ \| \tilde{p}(\cdot, t_i) - p_h(t_i) \|_{L^2(\Omega)} + \| p_h(t_i) - \bar{p}_h \|_{L^2(\Omega)},
\]

where the functions \( y_h \) and \( p_h \) are discretized in space with a finite element method.

**Remark 3.12** (Regularity). The order conditions in this section were taken from [3, 4, 8] and derived with techniques based on Taylor series. Therefore high regularity assumptions and smooth solutions are needed to observe these rates. For a reduction of the required regularity one might use generalized Taylor polynomials as in the work by Dupont and Scott [5], this is work of further research.

4. Numerical examples

After the classification of the Runge-Kutta schemes we consider in this section a numerical example which confirms the predicted convergence rates.

As in [1, 6] we solve the discretization (3) as a system of linear equation for the vector of unknowns

\[
(\bar{y}_h 1, \ldots, \bar{y}_h N, \bar{p}_h 0, \ldots, \bar{p}_h N, \bar{y}_h 0, 1, \ldots, \bar{y}_h N; s, \bar{p}_h 0; s, \ldots, \bar{p}_h N; s)^T.
\]

For the numerical examples we consider the optimal control problem

\[
\begin{align*}
\min \frac{1}{2} \| y(\cdot, T) - y_D \|_{L^2(\Omega)}^2 + \frac{\nu}{2} \int_0^T \| u \|_{L^2(\Omega)}^2 \, dt, \\
y(t) - \Delta y = u, & \quad \text{in } \Omega \times (0, T], \\
\frac{\partial y}{\partial n} = 0, & \quad \text{on } \partial \Omega \times (0, T], \\
y(\cdot, 0) = v, & \quad \text{in } \Omega,
\end{align*}
\]

(5)

with \( \Omega = (0, 1), T = 1 \) and \( y_D = v = \sqrt{2} \cos(\pi x) \).

**Remark 4.1.** (See also [6].) The analytic solution of the optimal control problem (1) with \( B = M = I \) and a self-adjoint elliptic operator \( A \) can be given as eigenfunction series (see [14]). Let \( \{ e_i \}_{i=0}^\infty \) and \( \{ \lambda_i \}_{i=0}^\infty \) be the series of eigenfunctions and eigenvalues of the spatial operator \( A \). If the data are given as eigenfunction expansions

\[
v = \sum_{k=0}^\infty y_0, k e_i, \quad y_D = \sum_{k=0}^\infty y_D, k e_i.
\]

(6)
Table 11: Coefficients for the exact solution (7) of the problem (5) to the data (6).

| $y_0,i$ | $y_D,i$ | $C_{1,i}$ | $C_{2,i}$ | $C_{3,i}$ |
|---------|---------|-----------|-----------|-----------|
| $a_i$   | $b_i$   | $-b_i + a_i e^{-\lambda_i}$ | $-b_i + a_i e^{\lambda_i} + 2\nu \lambda_i e^\lambda_i$ | $2\lambda_i \nu C_{1,i}$ |

The optimal control problem decouples into independent problems for every eigenfunction $e_i$ and has the solution

$$\bar{y} = \sum_{i=0}^{\infty} C_{1,i} e_i \e^{\lambda_i t} + C_{2,i} e_i \e^{-\lambda_i t}, \quad \bar{p} = \sum_{i=0}^{\infty} C_{3,i} e_i \e^{\lambda_i t}. \quad (7)$$

The coefficients can be computed with Maple and are given in Table 11.

For the example (5) with $y_D = v = \sqrt{2} \cos(\pi x)$ the series for the state and the adjoint state reduce to the terms with the second eigenfunction $e_1 = \sqrt{2} \cos(\pi x)$ of the Laplace operator with Neumann boundary conditions, i.e., only the coefficients $C_{1,1}$, $C_{2,1}$ and $C_{3,1}$ do not vanish.

The spatial discretization is adapted to the time discretization. The polynomial degree of the Lagrange finite elements for the spatial discretization is chosen as $k - 1$ for time discretization schemes of order $k$. So an error splitting argument provides the error bound

$$\| \bar{y}(\cdot, t_i) - \bar{y}_{hi} \|_{L^2(\Omega)} + \| \bar{p}(\cdot, t_i) - \bar{p}_{hi} \|_{L^2(\Omega)} \lesssim h^k + \tau^k.$$

In the numerical examples the discretization parameters $\tau$ and $h$ are chosen so that $\tau \sim h$.

We measure the time discretization error by the quantities

$$\max_{i \in \{0, 1, \ldots, N\}} \left( (\bar{y}_{hi} - I_h \bar{y}(x, t_i))^T M(\bar{y}_{hi} - I_h \bar{y}(x, t_i)) \right)^{\frac{1}{2}}, \quad (8)$$

$$\max_{i \in \{0, 1, \ldots, N\}} \left( (\bar{p}_{hi} - I_h \bar{p}(x, t_i))^T M(\bar{p}_{hi} - I_h \bar{p}(x, t_i)) \right)^{\frac{1}{2}}, \quad (9)$$

where $I_h$ is the Lagrangian interpolation operator to the corresponding spatial discretization and $M$ the finite element mass matrix. In Figure 1 to Figure 5 we observe nicely the predicted convergence rates for the example (5) with $\nu = 0.001$. In the computations with some fourth and sixth order schemes we also observe the influence of the round-off error due to the high numbers of unknowns. All the computations were done in Matlab.

The predicted order reduction for the SDIRK method can be seen in Figure 1b. For spatial discretization of the numerical example with the SDIRK time discretization cubic Lagrange finite elements are used, as for the other fourth order time discretization schemes.

Remark 4.2. The order reduction of the SDIRK method can also be observed for an optimal control problem with one linear ordinary differential equation. Consider the optimal control problem

$$\begin{align*}
\min \left\{ \frac{1}{2} (y(1) - 1)^2 + \frac{\nu}{2} \int_0^1 u^2 \,dt, \right. \\
y_t + \pi^2 y = u, \quad &\text{for } t \in (0, 1], \\
y(0) = 1. \left. \right\} \quad (10)
\end{align*}$$
(a) Second order convergence of the discretization based on the Störmer-Verlet discretization of Table 7a.

(b) Second order convergence of the discretization based on the SDIRK scheme of Table 8b.

Figure 1: Observed convergence order two of the numerical approximation of the example \(5\).

(a) Third order convergence of the discretization based on the Radau IA scheme of Table 7b.

(b) Third order convergence of the discretization based on the Radau IIA scheme of Table 7c.

Figure 2: Observed convergence order three of the numerical approximation of the example \(5\).
(a) Fourth order convergence of the discretization based on the Gauss scheme of Table 8a.
(b) Fourth order convergence of the discretization based on the Lobatto IIIA scheme of Table 8b.
(c) Fourth order convergence of the discretization based on the Lobatto IIIB scheme of Table 8c.
(d) Fourth order convergence of the discretization based on the Lobatto IIIC scheme of Table 8d.

Figure 3: Observed convergence order four of the numerical approximation of the example 5.
Even for this very simple example we observe the reduced convergence rate in Figure 4. Again the regularization parameter $\nu = 0.001$ was chosen.

**Remark 4.3.** The optimal control problem (10) can be interpreted as a spatial Galerkin discretization of optimal control Problem (5), where the bases of trial and test space are chosen as the second normalized eigenfunction of the Laplace operator. Note that the first eigenfunction of the Laplace operator with Neumann boundary conditions is the constant function.

**Remark 4.4.** In Figure 1a we observe the second order convergence of the Störmer-Verlet scheme. Similar observations were presented in [6]. But in contrast to [6], where the convergence of the state was observed in the time discretization points $t_i$ and the convergence of the adjoint state was observed in the time middle points $t_{i+\frac{1}{2}} = \frac{t_i + t_{i+1}}{2}$, we present in Figure 1a the convergence of the state and the adjoint state in the time discretization points $t_i$.

## 5. Conclusions and Outlook

In this paper we discussed the use of higher order implicit Runge-Kutta schemes for optimal control with parabolic partial differential equations for which optimization and discretization commute. In terms of the well known simplifying assumptions on the coefficients of implicit Runge-Kutta scheme we were able to give a classification for which discretization schemes up to order six the convergence order is preserved. For collocation schemes of Gauss, Radau IA, Radau IIA, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC type and a SDIRK scheme the expected and the numerical convergence rates coincide nicely.

For schemes of order higher than six the order conditions are not known explicitly, but they can be computed with the aid of bi-colored Butcher trees, as described in [3, 4]. For a reduction of the additional order conditions of order higher as six the procedure presented in
(a) Sixth order convergence of the discretization based on the three stage Gauss scheme.
(b) Sixth order convergence of the discretization based on the four stage Lobatto IIIA scheme.
(c) Sixth order convergence of the discretization based on the four stage Lobatto IIIB scheme.
(d) Sixth order convergence of the discretization based on the four stage Lobatto IIIC scheme.

Figure 5: Observed convergence order six of the numerical approximation of the example (5).
this paper is not practical due the huge number of additional conditions. Therefore a more elegant technique should be developed for the classification of schemes of order higher than six.

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A. Proof of Theorem 3.7

Full proof of Theorem 3.7. The idea of the proof is to use the simplifying assumptions \( B(p) \), \( C(\eta) \), \( D(\zeta) \) to reduce the additional order conditions to the classic order conditions or order conditions of lower order, which have already been reduced to the order conditions of the uncontrolled system. As all the numerical schemes fulfill the order conditions for the uncontrolled systems, these conditions can be used to calculate the value of the reduced expression.

Surely the way of the application of the simplifying assumptions is not unique, here one possibility is presented. A first goal in the reduction of order conditions with a fraction \( \frac{b_i}{b_j} \) is to use \( D(\zeta) \) to produce an additional \( b_i \) which cancels out. In the following we discuss the reduction of all the additional order conditions.

1. For the first additional order condition of \( A5-1 \) we use the simplifying assumption \( D(\zeta) \) for \( \zeta = 1 \), the last condition of \( O4 \) and the first condition of \( O5-3 \). This yields

\[
\sum_{kl} \frac{1}{b_{lk}} a_{lk} c_k d_k d_l = \sum_{kl} d_l a_{lk} c_k - \sum_{kl} a_{lk} c_k^2 d_l = \frac{1}{24} - \frac{1}{60} = \frac{1}{40}.
\]

2. For the second additional order condition of \( A5-1 \) we use the simplifying assumption \( D(\zeta) \) for \( \zeta = 1 \) and the third condition of \( O4 \) and the second condition of \( O5-3 \) to
get
\[ \sum_k \frac{1}{b_k} c_k^2 d_k^2 = \sum_k c_k^2 d_k - \sum_k c_k^3 d_k = \frac{1}{12} - \frac{1}{20} = \frac{1}{30}. \]

3. For the last order condition of (A5-1) we use again the simplifying assumption (D(ζ)) for ζ = 1, the first condition of (O3), the third condition of (O4) and the first condition of (O5-2). This gives
\[ \sum_l \frac{1}{b_l} c_l^2 d_l^3 = \sum_l c_l d_l^3 - 2 \sum_l c_l^2 d_l = \frac{1}{6} - \frac{2}{12} - \frac{1}{20} = \frac{1}{20}. \]

4. For the first condition of (A5-2) we apply the simplifying assumption (D(ζ)) for ζ = 1 and use the last condition of (O4) and the second condition of (O5-1), which gives
\[ \sum_{kl} \frac{1}{b_k} a_{kl} c_l^2 d_k^2 = \sum_{kl} a_{kl} c_l d_k - \sum_{kl} a_{kl} c_l d_k c_k = \frac{1}{24} - \frac{1}{40} = \frac{1}{60}. \]

5. For the second condition of (A5-2) we use the simplifying assumption (D(ζ)) for ζ = 1, the condition (O2), the first condition of (O3), the third condition of (O4) and the first condition of (O5-2) to end with
\[ \sum_m \frac{1}{b_m} d_m^4 = \sum_m d_m - \sum_m 3d_m c_m + \sum_m 3d_m c_m^2 - \sum_m d_m c_m^3 = \frac{1}{5}. \]

6. For the third condition of (A5-2) we apply the simplifying assumption (C(η)) for η = 2 twice and get with the second condition of (O5-3) the result
\[ \sum_{ijk} b_i a_{ik} a_{ij} c_j c_k = \sum_i b_i \left( \sum_k a_{ik} c_k \right) \left( \sum_j a_{ij} c_j \right) = \frac{1}{3} \sum_i b_i c_i^4 = \frac{1}{20}. \]

7. For the first condition of (A5-3) we apply again the simplifying assumption (C(η)) for η = 2 and the use of the first condition of (O5-3) yields
\[ \sum_{jkl} a_{lk} a_{kj} c_j d_l = \sum_{jkl} a_{lk} d_l \left( \sum_j a_{kj} c_j \right) = \frac{1}{2} \sum_{jkl} a_{lk} d_l c_k^2 = \frac{1}{120}. \]

8. For the second condition of (A5-3) we apply first the simplifying assumptions (D(ζ)) for η = 1 and then the definition of c_l and the simplifying assumption (C(η)) for η = 2. Together with the third condition of (O4) and the first condition of (O5-2) this gives
\[ \sum_{kl} \frac{1}{b_k} a_{lk} d_k c_l d_l = \sum_l c_l d_l \left( \sum_k a_{lk} \right) - \sum_l c_l d_l \left( \sum_k a_{lk} c_k \right) = \sum_l c_l^2 d_l - \frac{1}{2} \sum_l c_l^3 d_l = \frac{7}{120}. \]
9. For the last condition of (A5-3) we apply the simplifying assumption \( D(\zeta) \) for \( \eta = 2 \) twice and get with \( O(1) \), the second condition of \( O(2) \) and the second condition of \( O(5-3) \) the result

\[
\sum_{ijk} b jbja_{jk}a_{ik}cjcj = \sum_{jkl} b_{jk}a_{jk}c_j + \sum_i b_i a_{ik}c_i = \frac{1}{2} \sum_j \left( \sum_i b_i a_{ik}c_i \right) = \frac{1}{4} \sum_k b_k(1 - c_k)(1 - c_k^2) = \frac{1}{4} \sum_k \left( b_k - 2b_kc_k^2 + b_kc_k \right) = \frac{2}{15}.
\]

10. For the first condition of (A5-4) we use the simplifying assumption \( D(\zeta) \) for \( \eta = 1 \) and \( \eta = 2 \), the second condition of \( O(4) \), the second condition of \( O(3) \) and the second condition of \( O(5-3) \) to get

\[
\sum_{i} b_i a_{ik}c_i c_k = \sum_i b_i a_{ik}c_i c_k - \sum_i c_i^2 \left( \sum_i b_i a_{ik} c_k \right) = \frac{1}{8} - \frac{1}{2} \sum_i c_i^2 b_k(1 - c_k^2) = \frac{7}{120}.
\]

11. For the second condition of (A5-4) we use again the simplifying assumptions \( D(\zeta) \) for \( \eta = 1 \) and \( \eta = 2 \). The remaining expressions are treated with \( O(1) \), the simplifying condition \( B(p) \) for \( p = 2 \), the second condition of \( O(3) \), the first condition of \( O(4) \) and the second condition of \( O(5-3) \). This gives

\[
\sum_{i} b_j a_{id}c_i d_i = \sum_i b_i a_{id}c_i(1 - c_i)^2 = \sum_i (1 - c_i)^2 \left( \sum_i b_i c_i a_{id} \right) = \frac{1}{2} \sum_i b_i(1 - c_i)^2(1 - c_i^2) = \frac{3}{20}.
\]

12. For the last condition of (A5-4) we use first the simplifying assumptions \( D(\zeta) \) for \( \eta = 1 \) we get due to symmetry properties

\[
\sum_{lmk} \frac{1}{b_k} a_{mk}a_{lk}d_i d_m = \sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk}(1 - c_l)(1 - c_m)
\]

\[
= \sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk} - 2 \sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk}c_l + \sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk}c_l c_m. \quad (11)
\]

The last term is the third condition of (A5-3) and therefore we already know how to treat this term. On the first term of (11) we apply the simplifying assumptions \( D(\zeta) \) for \( \eta = 1 \) twice and get with \( O(1) \), \( B(p) \) for \( p = 2 \) and the second condition of \( O(3) \)

\[
\sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk} = \sum_k \frac{1}{b_k} \left( \sum_m b_m a_{mk} \right) \left( \sum_l b_l a_{lk} \right) = \sum_k b_k(1 - c_k)^2 = \frac{1}{3}.
\]

For the remaining term of (11) the use of \( D(\zeta) \) for \( \eta = 1 \) and \( \eta = 2 \) and \( O(1) \), \( B(p) \) for \( p = 2 \), the second condition of \( O(2) \) and the first condition of \( O(2) \) yields

\[
\sum_{lmk} \frac{b_m}{b_k} a_{mk}a_{lk}c_l = \sum_k \frac{1}{b_k} \left( \sum_m b_m a_{mk} \right) \left( \sum_l b_l a_{lk}c_l \right) = \frac{1}{2} \sum_k b_k(1 - c_k)(1 - c_k^2) = \frac{5}{24}.
\]
Altogether we have

$$\sum_{lmk} \frac{1}{b_k} a_{mk} a_{lk} d_k d_m = \frac{1}{3} - \frac{5}{12} + \frac{2}{15} = \frac{1}{20}.$$ 

13. For the first condition of (A5-5) we start with the use of the simplifying assumption (D(\(\zeta\))) for \(\eta = 1\) and the definition of \(c_m\). The last condition of (O4), the first condition of (O5-3) and the first condition of (O3) give

\[
\sum_{lm} \frac{1}{b_l} a_{ml} d_l^2 d_m = \sum_{lm} a_{ml}(1 - c_l)^2 d_m = \sum_{lm} a_{ml} d_m - 2 \sum_{lm} a_{ml} c_l d_m + \sum_{lm} a_{ml} d_m c_k^2
\]

\[
= \sum_{m} c_m d_m - \frac{1}{12} + \frac{1}{6} = \frac{1}{6} - \frac{1}{15} = \frac{1}{10}.
\]

14. For the second condition of (A5-5) the use of (D(\(\zeta\))) for \(\zeta = 1\), the definition of \(c_i\), the last condition of (O4), the simplifying assumption (C(\(\eta\))) for \(\eta = 2\) and the first condition of (O5-3) yields

\[
\sum_{kml} \frac{1}{b_i} a_{i k} c_l d_k d_m = \sum_{kml} a_{i k} a_{i k} d_m - \sum_{kml} a_{i k} a_{i k} d_m c_k
\]

\[
= \sum_{mld} a_{ml} c_l d_m - \sum_{mld} a_{ml} d_m \left( \sum_{k} a_{i k} c_k \right) = \frac{1}{24} - \frac{1}{2} \sum_{ml} a_{ml} d_m c_k^2
\]

\[
= \frac{1}{24} - \frac{1}{120} = \frac{1}{30}.
\]

15. For the last condition of (A5-5) we apply the simplifying assumption (D(\(\zeta\))) for \(\zeta = 2\), the definition of \(c_l\), first condition of (O5-3) and the first condition of (O3) to get

\[
\sum_{ikl} \frac{b_i}{b_k} a_{i k} a_{i k} c_l d_l = \sum_{ik} \frac{1}{b_k} a_{i k} d_l \left( \sum_{i} b_{i} a_{i k} c_i \right) = \frac{1}{2} \sum_{lk} a_{i k} d_l - \frac{1}{2} \sum_{lk} a_{i k} d_l c_k^2
\]

\[
= \frac{1}{2} \sum_{l} c_l d_l - \frac{1}{120} = \frac{3}{40}.
\]

16. For the first condition of (A5-6) we use the simplifying assumption (D(\(\zeta\))) for \(\zeta = 1\) and the simplifying assumption (C(\(\eta\))) for \(\zeta = 2\) three times. With the definition of \(c_i\), the first condition of (O4) and the second condition of (O5-3) we get

\[
\sum_{ikl} \frac{b_i}{b_k} a_{i k} a_{i l} d_k c_l = \sum_{ik} \frac{1}{b_k} a_{i k} \left( \sum_{i} a_{i l} c_l \right) - \sum_{ik} \frac{1}{b_i} \left( \sum_{k} a_{i k} c_k \right) \left( \sum_{l} a_{i l} c_l \right)
\]

\[
= \frac{1}{2} \sum_{i} b_{i} c_i^2 \left( \sum_{k} a_{i k} \right) - \frac{1}{4} \sum_{i} b_{i} c_i^4 = \frac{1}{2} \sum_{i} b_{i} c_i^3 - \frac{1}{20} = \frac{1}{8} - \frac{1}{20} = \frac{3}{40}.
\]

17. To the second condition of (A5-6) we apply the simplifying assumption (D(\(\zeta\))) for \(\zeta = 1\) once, use the definition of \(c_i\), the third condition of (A4) and the first condition of (A5-6).
This yields
\[
\sum_{ilm} b_i a_{im} a_{jd} d_m = \sum_{ilm} b_i a_{im} a_{jd} d_m - \sum_{ilm} b_i a_{im} a_{id} c_d d_m = \sum_{ilm} b_i a_{im} c_d d_m - \sum_{ilm} b_i a_{im} a_{id} c_d d_m = \frac{2}{15}.
\]

18. The application of the simplifying assumption \( [\text{D}(\zeta)] \) for \( \zeta = 1 \) to the last condition of (A5-6) together with the last condition of (O5-2), the definition of \( c_i \) and the first condition of (O4) gives
\[
\sum_{ik} b_i a_{ik} c_k^2 d_k = \sum_{ik} b_i a_{ik} c_k^2 - \sum_{ik} b_i a_{ik} c_k^2 c_k = \sum_{ik} b_i c_i^3 - \frac{1}{10} = \frac{3}{20}.
\]

19. For the condition (A5-7) we use the simplifying assumption \( [\text{D}(\zeta)] \) for \( \zeta = 1 \) two times, the definition of \( c_i \), the first condition of (O3), the third and fourth conditions of (O4) and the second condition of (O5-1) and get
\[
\sum_{lm} \frac{1}{b_j b_m} a_{lm} d_l^2 d_m = \sum_{lm} a_{lm} d_l - \sum_{lm} a_{lm} d_l c_l - \sum_{lm} a_{lm} d_l c_l c_m + \sum_{lm} a_{lm} d_l c_l c_m = \sum_{lm} c_l d_l - \sum_{lm} c_l^2 d_l - \sum_{lm} a_{lm} d_l c_l c_m + \sum_{lm} a_{lm} d_l c_l c_m = \frac{1}{15}
\]

Altogether we have derived the additional order conditions with the use of the simplifying assumptions and \( [\text{B}(p)] \) for \( p \leq 2 \), \( [\text{C}(\eta)] \) for \( \eta = 1, 2 \), \( [\text{D}(\zeta)] \) for \( \zeta = 1, 2 \), and the order conditions (O1)–(O4) and (O5-1)–(O5-3).

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