IMPLICIT-EXPLICIT RUNGE-KUTTA SCHEMES FOR NUMERICAL DISCRETIZATION OF OPTIMAL CONTROL PROBLEMS *

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Abstract. Implicit-explicit (IMEX) Runge-Kutta methods play a major rule in the numerical treatment of differential systems governed by stiff and non-stiff terms. This paper discusses order conditions and symplecticity properties of a class of IMEX Runge–Kutta methods in the context of optimal control problems. The analysis of the schemes is based on the continuous optimality system. Using suitable transformations of the adjoint equation, order conditions up to order three are proven as well as the relation between adjoint schemes obtained through different transformations is investigated. Conditions for the IMEX Runge–Kutta methods to be symplectic are also derived. A numerical example illustrating the theoretical properties is presented.

Key words. IMEX schemes, optimal control, symplectic methods, Runge-Kutta methods

AMS subject classifications. 65Kxx, 49M25, 65L06

1. Introduction. Recently, there has been intense research on the time discretization of optimal control problems involving differential equations. Such methods have found widespread applications in aerospace and mechanical engineering, the life sciences, and many other disciplines. In particular, properties of Runge–Kutta methods have been investigated for example in [10, 3, 16, 18, 12, 8, 9]. Hager [10] investigated order conditions (up to order four) for Runge–Kutta methods applied to optimality systems. This work has been later extended [3, 16] and also properties of symplecticity of the scheme have been studied, see also [6]. Further studies of discretizations of state and control constrained problems using Runge–Kutta methods have been conducted in [8, 9]. The observations lead to the idea to extend also other schemes like W-methods to optimal control problems [18]. Further, automatic differentiation has been applied to Runge–Kutta discretizations [24].

In many practical application involving systems of differential equations of the form

$$y'(t) = f(y(t), t) + g(y(t), t),$$

where f and g are eventually obtained as suitable finite-difference or finite-element approximations of spatial derivatives, the time scales induced by the two operators may be considerably different. Let us assume that f is the non-stiff term and g the stiff one. Although the problem is stiff as a whole, the use of fully implicit solvers originates a nonlinear system of equations involving also the non-stiff term f which quite often represent the most expensive/difficult term in the computation. Thus it is highly desirable to have a combination of implicit and explicit (IMEX) discretization terms to resolve stiff and non-stiff dynamics accordingly. For Runge-Kutta methods

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such schemes have been studied in [1, 4, 5, 7, 14, 17, 20, 19]. Among the prominent examples are the numerical integration of hyperbolic conservation laws, convection–diffusion equations and singular perturbed problems.

As discussed in [17, 20] the construction of such methods implies new difficulties due to the appearance of coupled order conditions and to the possible loss of accuracy close to stiff regimes. The present work is concerned with the use of implict–explicit methods in the context of optimal control problems. Here we focus our attention to the order condition of the adjoint IMEX system and its symplecticity property leaving to further research specific application to partial differential equations. We refer to [2, 12] for examples of applications to hyperbolic problems.

The general IMEX Runge-Kutta scheme is introduced in Section 2 as well as its discrete adjoint equations. A transformation of these equations is proposed in order to later on analyse order conditions and symplecticity properties. Since the presented transformation is different from the one used for example in [10, 12] we also discuss the relation between the schemes obtained by using the different transformations. The existing relations are summarized in Figure 2.1. We furthermore investigate the relation between the two possible approaches to derive the optimality system: we prove in Theorem 2.1 that discretize-then-optimize and optimize-then-discretize are equivalent. The order conditions up to order three are summarized in Theorem 3.1 and the results on symplecticity are given in Theorem 3.2. A numerical example is presented in Section 4. Examples of IMEX Runge-Kutta schemes up to order three are reported in a separate appendix.

2. IMEX Runge-Kutta methods for optimal control problems.

2.1. The optimal control problem. We consider optimal control problems for ordinary differential equations of type (2.1):

$$(OCP)$$
 min $j(y(T))$ such that (2.1a)

$$\dot{y}(t) = f(y(t), u(t)) + g(y(t), u(t)), \qquad t \in [0, T]$$
 (2.1b)

$$y(0) = y^0.$$
 (2.1c)

Related to the optimal control problem we introduce the Hamiltonian function H as $H(y, u, p) := p^T(f(y, u) + g(y, u))$. Under appropriate conditions it is well-known [13, 23] that the first-order optimality conditions for (2.1) are

$$\dot{y} = H_p(y, u, p) = f(y, u) + g(y, u), \qquad y(0) = y^0$$
 (2.2a)

$$\dot{p} = -H_y(y, u, p) = -f_y(y, u)^T p - g_y(y, u)^T p, \qquad p(T) = j'(y(T))$$
 (2.2b)

$$0 = H_u(y, u, p) = f_u(y, u)^T p + g_u(y, u)^T p.$$
(2.2c)

The equation (2.2a) is called state equation and (2.2b) is called adjoint equation. We are interested in implicit–explicit Runge–Kutta (IMEX–RK) discretizations for (2.2a) and (2.2b). To be more precise, we treat f by an explicit method and assume that g enjoys some stiffness so that an implicit method is required. Therefore, the discretization of the general case of (2.2a) leads to two different schemes for f and g, respectively. A corresponding Runge-Kutta discretization scheme [19, 20] with s stages is given by

$$Y_n^{(i)} = y_n + h \sum_{j=1}^s \tilde{a}_{ij} f(Y_n^{(j)}, u_n^j) + h \sum_{j=1}^s a_{ij} g(Y_n^{(j)}, u_n^j) \qquad i = 1, .., s$$
(2.3a)

$$y_{n+1} = y_n + h \sum_{i=1}^s \tilde{\omega}_i f(Y_n^{(i)}, u_n^i) + h \sum_{i=1}^s \omega_i g(Y_n^{(i)}, u_n^i), \qquad n = 0, 1, 2, .$$
(2.3b)

where $A, \tilde{A}, \omega, \tilde{\omega}$ are the associated Runge–Kutta coefficient matrices and the Runge– Kutta weights, respectively. We refer to methods where an explicit scheme for f and an implicit scheme for g is used as as IMEX–RK schemes. Their properties have been investigated for example in [1, 19, 20]. A particularly interesting subclass is the class of diagonally implicit IMEX–RK methods.

DEFINITION 2.1. We call the method (2.3) diagonally implicit IMEX-RK method, iff $\tilde{a}_{ij} = 0$ for $j \ge i$ and $a_{ij} = 0$ for all j > i.

In order to simplify the notation in the sequel we do not truncate the corresponding sums and, if not stated otherwise, all following results are given for a general implicit–explicit methods. Only later we will reduce the investigation to the class of diagonally implicit methods.

As in [3, 20, 19] we use an equivalent formulation of the IMEX–RK scheme in order to derive the discrete first–order optimality conditions. Instead of representation (2.3) we use the equivalent formulation (2.4)

$$\tilde{K}_{n}^{(i)} = f\left(y_{n} + h\sum_{j=1}^{s} \tilde{a}_{ij}\tilde{K}^{(j)} + h\sum_{j=1}^{s} a_{ij}K_{n}^{(j)}, u_{n}^{i}\right)$$
(2.4a)

$$K_n^{(i)} = g\left(y_n + h\sum_{j=1}^s \tilde{a}_{ij}\tilde{K}^{(j)} + h\sum_{j=1}^s a_{ij}K_n^{(j)}, u_n^i\right)$$
(2.4b)

$$y_{n+1} = y_n + h \sum_{i=1}^s \tilde{\omega}_i \tilde{K}_n^{(i)} + h \sum_{i=1}^s \omega_i K_n^{(i)}.$$
 (2.4c)

Note that due to the two different schemes for f and g, respectively, we introduce two auxiliary variables $\tilde{K}^{(i)}$ and $K^{(i)}$. These lead to additional discrete adjoint equations compared with the formulation in [3]. The associated discretized optimal control problem to (2.1) using IMEX–RK is hence given by

$$(DOP) \quad \min j(y_N) \text{ such that}$$
 (2.5a)

$$\tilde{K}^{(i)} = f\left(y_n + h\sum_{j=1}^s \tilde{a}_{ij}\tilde{K}^{(j)} + h\sum_{j=1}^s a_{ij}K^{(j)}, u_n^i\right)$$
(2.5b)

$$K^{(i)} = g\left(y_n + h\sum_{j=1}^s \tilde{a}_{ij}\tilde{K}^{(j)} + h\sum_{j=1}^s a_{ij}K^{(j)}, u_n^i\right)$$
(2.5c)

$$y_{n+1} = y_n + h \sum_{i=1}^{s} \tilde{\omega}_i \tilde{K}^{(i)} + h \sum_{i=1}^{s} \omega_i K^{(i)}, \quad y_0 = y^0.$$
 (2.5d)

Clearly, the Lagrangian is

$$\mathcal{L}(y, K, \tilde{K}, p, \tilde{\xi}, \xi) = j(y_N) + p_0^T(y_0 - y^0) + \sum_{n=0}^{N-1} \left[p_{n+1}^T \left(-y_{n+1} + y_n + h \sum_{i=1}^s \tilde{\omega}_i \tilde{K}_n^{(i)} + h \sum_{i=1}^s \omega_i K_n^{(i)} \right) + \sum_{i=1}^s (\tilde{\xi}_n^{(i)})^T (-\tilde{K}_n^{(i)} + f(Y_n^{(i)}, u_n^i)) + \sum_{i=1}^s (\xi_n^{(i)})^T (-K_n^{(i)} + g(Y_n^{(i)}, u_n^i)) \right]$$
(2.6)

where $Y_n^{(i)} := y_n + h \sum_{j=1}^s \tilde{a}_{ij} \tilde{K}_n^{(j)} + h \sum_{j=1}^s a_{ij} K_n^{(j)}$. Here, the vectors $\tilde{\xi}, \xi$ and p are the Lagrange multipliers corresponding to the equality constraints given by the initial condition and system (2.4), respectively. For the first order necessary optimality conditions for (2.5) we obtain the feasibility conditions given by (2.4) and furthermore the discrete adjoint equations which are derived upon differentiation of $\mathcal{L}(y, p, \tilde{\xi}, \xi)$ with respect to $K_n^{(i)}, \tilde{K}_n^{(i)}$ and y_n , respectively. The system of adjoint equations reads

$$\tilde{\xi}_{n}^{(i)} = h \,\tilde{\omega}_{i} \, p_{n+1} + h \sum_{j=1}^{s} \tilde{a}_{ji} \, f_{y} (Y_{n}^{(j)}, u_{n}^{j})^{T} \tilde{\xi}_{n}^{(j)} + h \sum_{j=1}^{s} \tilde{a}_{ji} \, g_{y} (Y_{n}^{(j)}, u_{n}^{j})^{T} \xi_{n}^{(j)} \quad (2.7a)$$

$$\xi_n^{(i)} = h \,\omega_i \, p_{n+1} + h \sum_{j=1}^s a_{ji} \, f_y (Y_n^{(j)}, u_n^j)^T \tilde{\xi}_n^{(j)} + h \sum_{j=1}^s a_{ji} \, g_y (Y_n^{(j)}, u_n^j)^T \xi_n^{(j)} \quad (2.7b)$$

$$p_n = p_{n+1} + \sum_{i=1}^s f_y(Y_n^{(i)}, u_n^i)^T \tilde{\xi}_n^{(i)} + \sum_{i=1}^s g_y(Y_n^{(i)}, u_n^i)^T \xi_n^{(i)}, \quad p_N = j'(y_N), (2.7c)$$

where the index range for n is N-1,..,0 and the intermediate adjoint states have to be computed for i = 1,..,s. The discretization method (2.7) is not yet in a standard RK notation. Similar to [3, 10, 12] we have the following result.

PROPOSITION 2.1. If we assume that $\tilde{\omega}_i \neq 0$ and $\omega_i \neq 0$ then (2.7) can be rewritten as

$$\tilde{P}^{(i)} = p_n - h \sum_{j=1}^s \tilde{\alpha}_{ij} f_y (Y_n^{(j)}, u_n^j)^T \tilde{P}^{(j)} - h \sum_{j=1}^s \alpha_{ij} g_y (Y_n^{(j)}, u_n^j)^T P^{(j)}$$
(2.8a)

$$P^{(i)} = p_n - h \sum_{j=1}^s \tilde{\beta}_{ij} f_y(Y_n^{(j)}, u_n^j)^T \tilde{P}^{(j)} - h \sum_{j=1}^s \beta_{ij} g_y(Y_n^{(j)}, u_n^j)^T P^{(j)}$$
(2.8b)

$$p_{n+1} = p_n - h \sum_{i=1}^s \tilde{\omega}_i f_y (Y_n^{(i)}, u_n^i)^T \tilde{P}^{(i)} - h \sum_{i=1}^s \omega_i g_y (Y_n^{(i)}, u_n^i)^T P^{(i)}, \quad (2.8c)$$

where the coefficients $\tilde{\alpha}_{ij}, \alpha_{ij}, \tilde{\beta}_{ij}$ and β_{ij} are given by

$$\tilde{\alpha}_{ij} := \tilde{\omega}_j - \frac{\tilde{\omega}_j}{\tilde{\omega}_i} \tilde{a}_{ji}, \quad \alpha_{ij} := \omega_j - \frac{\omega_j}{\tilde{\omega}_i} \tilde{a}_{ji}, \quad \tilde{\beta}_{ij} := \tilde{\omega}_j - \frac{\tilde{\omega}_j}{\omega_i} a_{ji}, \quad \beta_{ij} := \omega_j - \frac{\omega_j}{\omega_i} a_{ji}.$$

Proof. If $\tilde{\omega}_i \neq 0$ and $\omega_i \neq 0$, then we can define new variables

$$\tilde{P}_{n}^{(i)} := \frac{\tilde{\xi}_{n}^{(i)}}{h\,\tilde{\omega}_{i}} \qquad \text{and} \qquad P_{n}^{(i)} := \frac{\xi_{n}^{(i)}}{h\,\omega_{i}} \qquad (i = 1, .., s; \quad n = 0, .., N - 1).$$
(2.9)

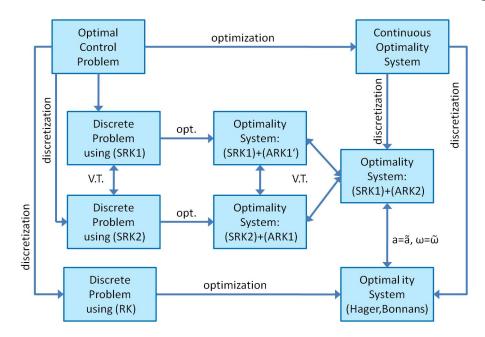


FIG. 2.1. Diagram summarizing the relations discussed. Here "V.T." stands for "variable transformation", (RK) denotes the single RK method for (2.2a) as in [3, 10], (SRK1) denotes system (2.3), (SRK2) denotes system (2.4), (ARK1) denotes system (2.7), (ARK2) denotes system (2.8) and (ARK1') denotes the discrete adjoint system (2.11).

We obtain (2.8) using the definition of $P_n^{(i)}$ and $\tilde{P}_n^{(i)}$ in $\xi_n^{(i)}$ and $\tilde{\xi}_n^{(i)}$, respectively.

REMARK 2.1. Referring to the classification of IMEX-RK methods given in [5], Proposition 2.1 is extended to IMEX schemes of type ARS with $\omega_1 = 0$. In this case, define $P_n^{(i)}$ for i = 2, ..., s and $\tilde{P}_n^{(i)}$ for i = 1, ..., s as in (2.9) and use the transformation to obtain (2.8a) and (2.8b) for i = 1, ..., s and i = 2, ..., s, respectively, and for the further equation we set

$$P_n^{(1)} := p_n - h \sum_{i=1}^s \tilde{\omega}_i f_y(Y_n^{(i)}, u_n^i)^T \tilde{P}^{(i)} - h \sum_{i=1}^s \omega_i g_y(Y_n^{(i)}, u_n^i)^T P^{(i)}$$

i.e. we use again (2.8b) and define the coefficients $\tilde{\beta}_{1j} := \tilde{\omega}_j$ and $\beta_{1j} := \omega_j$. The remaining coefficients are defined as in Proposition 2.1.

2.2. Discrete and continuous optimality systems. We prove the following results on the relations depicited in Figure 2.1. The discrete optimality system of (2.5) represents a RK discretization of the continuous optimality system (2.2). The system obtained by discretizing the continuous optimality system (2.1) and by optimizing the discretized optimal control problem coincide.

THEOREM 2.1. We consider the first-order necessary optimality conditions (2.2) of the optimal control problem (2.1).

The equations (2.3) and (2.8) are the discrete state and adjoint equations of the optimality system to the problem $\min j(y_N)$ subject to (2.3).

The equations (2.3) and (2.8) are a discretization of the continuous state (2.2a) and adjoint (2.2b) equation.

The proof of Theorem 2.1 follows showing that system (2.3) yields a discretization scheme (2.11) for (2.2b) and the latter is transformed into (2.8) by a variable transformation of the intermediate states.

LEMMA 2.1. Given the optimal control problem (2.1) and the RK discretization (2.3) for the state equation (2.2a). Then, the associated RK discretization of the discrete adjoint equation is equivalent to (2.8).

Proof. The associated discretized optimal control problem is given by

$$(DOP_1) \quad \min j(y_N) \tag{2.10a}$$

$$Y_n^{(i)} = y_n + h \sum_{j=1}^s \tilde{a}_{ij} f(Y_n^{(j)}, u_n^j) + h \sum_{j=1}^s a_{ij} g(Y_n^{(j)}, u_n^j),$$
(2.10b)

$$y_{n+1} = y_n + h \sum_{i=1}^{s} \tilde{\omega}_i f(Y_n^{(i)}, u_n^i) + h \sum_{i=1}^{s} \omega_i g(Y_n^{(i)}, u_n^i), \quad y_0 = y^0.$$
(2.10c)

The stationary points of the Lagrangian yield for $i = 1, \ldots, s$ and $n = 1, \ldots, N-1$

$$\zeta_n^{(i)} = h \left(\tilde{\omega}_i f_y(Y_n^{(i)}, u_n^i) + \omega_i g_y(Y_n^{(i)}, u_n^i) \right)^T p_{n+1}$$
(2.11a)

$$+\sum_{j=1}^{s} \tilde{a}_{ji} f_y(Y_n^{(i)}, u_n^i)^T \zeta^{(j)} + h \sum_{j=1}^{s} a_{ji} g_y(Y_n^{(i)}, u_n^i)^T \zeta^{(j)}$$
(2.11b)

$$p_n = p_{n+1} + \sum_{i=1}^{s} \zeta_n^{(i)}, \quad p_N = j'(y_N)$$
 (2.11c)

$$0 = h \left(\tilde{\omega}_i f_u(Y_n^{(i)}, u_n^i) + \omega_i g_u(Y_n^{(i)}, u_n^i) \right)^T p_{n+1}$$
(2.11d)

$$+\sum_{j=1}^{s} \tilde{a}_{ji} f_u(Y_n^{(i)}, u_n^i)^T \zeta^{(j)} + h \sum_{j=1}^{s} a_{ji} g_u(Y_n^{(i)}, u_n^i)^T \zeta^{(j)}$$
(2.11e)

The system (2.11) is not in a standard RK formulation. As in [10, 12] we reformulate this system as a standard partitioned RK method for p. In contrast to [10] we introduce two new variables:

$$\tilde{P}_{n}^{(i)} := p_{n+1} + \sum_{j=1}^{s} \frac{\tilde{a}_{ji}}{\tilde{\omega}_{i}} \zeta_{n}^{(j)} \quad \text{and} \quad P_{n}^{(i)} := p_{n+1} + \sum_{j=1}^{s} \frac{a_{ji}}{\omega_{i}} \zeta_{n}^{(j)}, \quad (2.12)$$

for all i = 1, ..., s and n = 0, ..., N - 1. Then, (2.11), yields the equivalent formulation of (2.8) with coefficients

$$\check{\alpha}_{ij} := \frac{\tilde{\omega}_j}{\tilde{\omega}_i} \tilde{a}_{ji}, \quad \hat{\alpha}_{ij} := \frac{\omega_j}{\tilde{\omega}_i} \tilde{a}_{ji}, \quad \check{\beta}_{ij} := \frac{\tilde{\omega}_j}{\omega_i} a_{ji}, \quad \hat{\beta}_{ij} := \frac{\omega_j}{\omega_i} a_{ji}.$$

Rewriting the resulting backward scheme as a forward scheme then yields (2.8).

LEMMA 2.2. Assume the optimal control problem (2.1) and the RK discretization scheme (2.3) for the state equation (2.2a) are given. The discrete state and adjoint equation (2.3) and (2.8), respectively, are equivalent to a RK discretization of the continuous optimality system (2.2).

Proof. Note that adding a corresponding set of equalities for \hat{p} , the system (2.3) together with (2.8) corresponds to a standard additive RK scheme for the extended

(modified) system with $\tilde{p}(T) = p(T)$ and

$$\dot{y} = f(y, u) + g(y, u)$$
 (2.13a)

$$\dot{\tilde{p}} = f_y(y, u)^T \tilde{p} + g_y(y, u)^T p \tag{2.13b}$$

$$\dot{p} = f_u(y, u)^T \tilde{p} + g_u(y, u)^T p \tag{2.13c}$$

The system (2.3) and (2.8) form an additive RK method for (2.13). Since \tilde{p} and p have the same initial conditions, we have $\tilde{p} \equiv p$. Therefore the solution to (2.13b) and (2.13c) are equivalent to the solution to (2.2b). Finally, the approximate adjoints p_h and \tilde{p}_h are the discretized solution to (2.2b) for the same initial equations. \Box

Theorem 2.1 follows directly by Lemma 2.1 and Lemma 2.2. We have a few comments on the implications of the previous theorem.

In view of (2.8), we obtain four additional RK coefficient matrices and therefore four RK methods. Furthemore, we have the two RK methods for the IMEX discretization (2.3). If we additionally assume that $\omega_i = \tilde{\omega}_i$ holds for all i = 1, ..., s, then we obtain $\tilde{\alpha}_{ij} = \alpha_{ij}$ and $\tilde{\beta}_{ij} = \beta_{ij}$ for all i, j = 1, ..., s. Hence we obtain only two additional RK schemes for the optimality system (2.2). Moreover, the equation is independent of the discretization of (2.2a). This implies that either (*DOP*) or (*DOP*₁) can be used to discretize the problem.

Also, if the Runge–Kutta methods for f and g coincide, i.e. $\tilde{a}_{ij} = a_{ij}$ and $\tilde{\omega}_i = \omega_i$ for all i, j, then the discrete adjoint scheme (2.8) coincides with the one derived by Hager [10] and it also coincides with Bonnans et al [3], respectively. We therefore recover their results. If $g \equiv 0$, then an explicit RK method for f in (2.3) yields a "backward" explicit method for (2.7) and an implicit method for (2.8). Here, the variables $\xi_n^{(i)}$ and $P_n^{(i)}$ vanish since there is no contribution to p_n and p_{n+1} , respectively. If $f \equiv 0$, then the backward variant of (2.8) yields a "backward" diagonally implicit method for g.

The system (2.7) is a "backward in time" scheme for the adjoint variable p, with initial value $j'(y_N)$. Note that if (2.3) is an implicit-explicit (IMEX) RK scheme with a diagonally implicit method (DIRK) for g, then (2.7) also is an IMEX method with a diagonally implicit method for the terms that belong to g. Hence, the presentation simplifies in this case which also has been discussed in [12]. Although (2.8) is more suitable for theoretical investigations, for an efficient implementation of the scheme we used formulation (2.7).

The discretization of equation (2.2c) is straight-forward

$$\tilde{\omega}_k f_u (Y_n^{(k)}, u_n^k)^T \tilde{P}_n^{(k)} + \omega_k g_u (Y_n^{(k)}, u_n^k)^T P_n^{(k)} = 0.$$
(2.14)

Next, we prove that for a suitable discretization $H^h(y_n, p_{n+1}, u_n)$ of the Hamiltonian H(y, p, u) (2.14) is equal to $\nabla_{u_k} H^h(y_n, p_{n+1}, u_n) = 0$. Hence, Lemma 2.3 shows that (2.14) is a valid discretization of $H_u(y, p, u) = 0$ in the limit $h \to 0$.

Lemma 2.3. Let

$$H^{h}(y_{n}, p_{n+1}, u_{n}) := p_{n+1}^{T} \left[\sum_{i=1}^{s} (\tilde{\omega}_{i} f^{(i)} + \omega_{i} g^{(i)}) \right]$$

with $f^{(i)} := f(Y_n^{(i)}, u_n^i)$ and $g^{(i)} := g(Y_n^{(i)}, u_n^i)$. Then,

$$\nabla_{u_k} H^h(y_n, p_{n+1}, u_n) = \tilde{\omega}_k (f_u^{(k)})^T \tilde{P}_n^{(k)} + \omega_k (g_u^{(k)})^T P_n^{(k)}$$

with $f_u^{(k)} := f_u(Y_n^{(k)}, u_n^k)$ and $g_u^{(k)} := g_u(Y_n^{(k)}, u_n^k)$.

Proof. In order to simplify the notation, we introduce the following matrices

$$\begin{split} B: s \times s \text{ block matrix with block entries } &(i,j) : [\tilde{a}_{ji}(f_y^{(i)})^T + a_{ji}(g_y^{(i)})^T], \qquad i,j=1,..,s \\ C: s \times 1 \text{ block matrix with block entries } &: [\tilde{\omega}_i(f_y^{(i)})^T + \omega_i(g_y^{(i)})^T], \qquad i=1,..,s \\ \tilde{D}_k: 1 \times s \text{ block matrix with block entries } &: [\tilde{a}_{ik}\mathbf{Id}], \qquad i=1,..,s \\ D_k: 1 \times s \text{ block matrix with block entries } &: [a_{ik}\mathbf{Id}], \qquad i=1,..,s \end{split}$$

with $f_y^{(i)} := f_y(Y_n^{(i)}, u_n^i)$ and $g_y^{(i)} := g_y(Y_n^{(i)}, u_n^i)$. Moreover, define $M := (\mathbf{Id} - hB)$ and note that M is invertible if h is sufficiently small. Using the just defined matrices, we rewrite (2.11a) as

$$M\zeta_n = hCp_{n+1} \tag{2.15}$$

where $\zeta_n = ((\zeta_n^{(1)})^T, ..., (\zeta_n^{(s)})^T)^T$ and the equations of (2.12) are

$$\tilde{\omega}_k \tilde{P}_n^{(k)} = \tilde{\omega}_k p_{n+1} + \tilde{D}_k \zeta_n$$
 and $\omega_k P_n^{(k)} = \omega_k p_{n+1} + D_k \zeta_n.$ (2.16)

Furthermore, differentiating (2.3) with respect to u_k yields

$$\nabla_{u_k} Y_n M = h(f_u^{(k)})^T \tilde{D}_k + h(g_u^{(k)})^T D_k, \qquad (2.17)$$

where $Y_n = ((Y_n^{(1)})^T, ..., (Y_n^{(s)})^T)^T$. Now, we use (2.15), (2.16) and (2.17) and evaluate the gradient of $H^h(y_n, p_{n+1}, u_n)$ with respect to u_k

$$\nabla_{u_{k}}H^{h}(y_{n}, p_{n+1}, u_{n}) = \sum_{i=1}^{s} \left(\tilde{\omega}_{i} \nabla_{u_{k}} Y_{n}^{(i)}(f_{y}^{(i)})^{T} p_{n+1} + \omega_{i} \nabla_{u_{k}} Y_{n}^{(i)}(g_{y}^{(i)})^{T} p_{n+1} \right) + \tilde{\omega}_{k}(f_{u}^{(k)})^{T} p_{n+1} + \omega_{k}(g_{u}^{(k)})^{T} p_{n+1} \\ = \nabla_{u_{k}} Y_{n} C p_{n+1} + \tilde{\omega}_{k}(f_{u}^{(k)})^{T} p_{n+1} + \omega_{k}(g_{u}^{(k)})^{T} p_{n+1} \\ = \left(h(f_{u}^{(k)})^{T} \tilde{D}_{k} + h(g_{u}^{(k)})^{T} D_{k} \right) M^{-1} C p_{n+1} + \tilde{\omega}_{k}(f_{u}^{(k)})^{T} p_{n+1} + \omega_{k}(g_{u}^{(k)})^{T} p_{n+1} \\ = (f_{u}^{(k)})^{T} (\tilde{D}_{k} \zeta_{n} + \tilde{\omega}_{k} p_{n+1}) + (g_{u}^{(k)})^{T} (D_{k} \zeta_{n} + \omega_{k} p_{n+1}) \\ = \tilde{\omega}_{k}(f_{u}^{(k)})^{T} \tilde{P}_{n}^{(k)} + \omega_{k}(g_{u}^{(k)})^{T} P_{n}^{(k)}.$$

3. Properties of the IMEX Runge-Kutta discretizations. Theoretical properties of the derived RK method for system (2.2) corresponding to the partitioned RK method are considered.

3.1. Order conditions. We analyse the order conditions for the RK method (2.3) together with (2.8). As in the proof of Lemma 2.2 we add the additional equation

$$\tilde{p}_{n+1} = \tilde{p}_n - h \sum_{i=1}^s \tilde{\omega}_i f_y (Y_n^{(i)}, u_n^i)^T \tilde{P}^{(i)} - h \sum_{i=1}^s \omega_i g_y (Y_n^{(i)}, u_n^i)^T P^{(i)},$$
(3.1)

for \tilde{p} such that the resulting method corresponds to a standard additive RK scheme for the auxiliary problem (2.13). Since the system is completely coupled, we also obtain a similar coupling in the order conditions [17].

We start with the analysis of first and second order conditions in the general case, i.e. $A \neq \tilde{A}$ and $\omega \neq \tilde{\omega}$. We then restrict ourselves to the case $\tilde{\omega} = \omega$. In this case all additional coupling conditions for first and second order are directly satisfied by the order condition for the forward IMEX scheme (2.3). For third order we obtain an additional condition. If we consider the adjoint equation alone those conditions have been studied in [12] for a decoupled system (2.3), (2.8).

Define the coefficients

$$c_i := \sum_{j=1}^s a_{ij}, \ \tilde{c}_i := \sum_{j=1}^s \tilde{a}_{ij}, \ \gamma_i := \sum_{j=1}^s \alpha_{ij}, \ \tilde{\gamma}_i := \sum_{j=1}^s \tilde{\alpha}_{ij}, \ \delta_i := \sum_{j=1}^s \beta_{ij}, \ \tilde{\delta}_i := \sum_{j=1}^s \tilde{\beta}_{ij},$$

and

$$d_j = \sum_{i=1}^s \omega_i \tilde{a}_{ij}, \quad \tilde{d}_j = \sum_{i=1}^s \tilde{\omega}_i \tilde{a}_{ij}, \quad e_j = \sum_{i=1}^s \omega_i a_{ij} \quad \text{and} \quad \tilde{e}_j = \sum_{i=1}^s \tilde{\omega}_i a_{ij}.$$

PROPOSITION 3.1. Consider the additive Runge-Kutta method (2.3) together with (2.8) and (3.1) as a discretization scheme for (2.13). For (2.3) consider a diagonally implicit IMEX-RK method. Then the following results hold true.

- 1. The additive method is of first order, if the diagonally implicit IMEX-RK method (2.3) is of first order.
- 2. The additive method is of second order, if the diagonally implicit IMEX-RK method (2.3) is of second order and it additionally satisfies the following coupling conditions

$$\sum_{i=1}^{s} \frac{\omega_i}{\tilde{\omega}_i} d_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \frac{\omega_i}{\tilde{\omega}_i} \tilde{d}_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \frac{\tilde{\omega}_i}{\omega_i} e_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \frac{\tilde{\omega}_i}{\omega_i} \tilde{e}_i = \frac{1}{2}.$$
(3.2)

Proof. The first part of the theorem is trivial. For the second part we prove

$$\sum_{i=1}^{s} \omega_i \gamma_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \omega_i \delta_i = \frac{1}{2}.$$

By the second order of the IMEX–RK method (2.3) and the definition of γ_i we have

$$\sum_{i=1}^{s} \tilde{\omega}_i \, \gamma_i = \sum_{i=1}^{s} \tilde{\omega}_i - \sum_{i=1}^{s} \sum_{j=1}^{s} \omega_j a_{ij} = 1 - \sum_{i=1}^{s} w_j \, \tilde{c}_j = \frac{1}{2}.$$

In the same way we prove that

$$\sum_{i=1}^{s} \tilde{\omega}_i \, \tilde{\gamma}_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \omega_i \, \delta_i = \frac{1}{2} \qquad \text{and} \qquad \sum_{i=1}^{s} \omega_i \, \tilde{\delta}_i = \frac{1}{2}$$

hold, if the second order conditions for (2.3) are satisfied. However, since the remaining coupling conditions cannot be simplified in the same way, we need to impose further the conditions (3.2). By (3.2) we get

$$\sum_{i=1}^{s} \omega_i \gamma_i = 1 - \sum_{i=1}^{s} \omega_i \left(\sum_{j=1}^{s} \frac{\omega_j}{\tilde{\omega}_i} \tilde{a}_{ji} \right) = 1 - \sum_{i=1}^{s} \frac{\omega_i}{\tilde{\omega}_i} d_i = \frac{1}{2}.$$

Accordingly, the remaining conditions hold true

$$\sum_{i=1}^{s} \omega_i \, \tilde{\gamma}_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} \tilde{\omega}_i \, \delta_i = \frac{1}{2} \qquad \text{and} \qquad \sum_{i=1}^{s} \tilde{\omega}_i \, \tilde{\delta}_i = \frac{1}{2}$$

.

The order conditions apply to all variables y, p and \tilde{p} and therefore y and p satisfy in particular equation (2.2). Moreover, if $\omega_i = \tilde{\omega}_i$ for all i = 1, ..., s then the additional second order conditions (3.2) are satisfied.

COROLLARY 3.1. If $\omega_i = \tilde{\omega}_i$ for all i = 1, ..., s and the diagonally implicit IMEX-RK method (2.3) is of second order, then the additive RK method (2.3) together with (2.8) and (3.1) is of second order.

Proof. Since,

$$\sum_{j=1}^{s} d_j = \sum_{i,j=1}^{s} \omega_j \tilde{a}_{ji} = \sum_{j=1}^{s} \omega_j \sum_{i=1}^{s} \tilde{a}_{ji} = \sum_{j=1}^{s} \omega_j \tilde{c}_j = \frac{1}{2}$$
(3.3)

and in the same way

$$\sum_{j=1}^{s} \tilde{d}_j = \frac{1}{2}, \qquad \sum_{j=1}^{s} e_j = \frac{1}{2} \qquad \text{and} \qquad \sum_{j=1}^{s} \tilde{e}_j = \frac{1}{2},$$

the conditions of (3.2) hold. \Box

THEOREM 3.1. If $\omega_i = \tilde{\omega}_i$ for all i = 1, ..., s and the diagonally implicit IMEX-RK method (2.3) is of third order, then the additive RK method (2.3) together with (2.8) and (3.1) is of third order, provided that

$$\sum_{i=1}^{s} \frac{d_i^2}{\omega_i} = \frac{1}{3}, \qquad \sum_{i=1}^{s} \frac{e_i^2}{\omega_i} = \frac{1}{3} \qquad and \qquad \sum_{i=1}^{s} \frac{d_i e_i}{\omega_i} = \frac{1}{3}$$
(3.4)

is satisfied.

Proof. If $\omega_i = \tilde{\omega}_i$ for all i = 1, ..., s, it follows that $\alpha_{ij} = \tilde{\alpha}_{ij}$ and $\beta_{ij} = \tilde{\beta}_{ij}$ for all i, j = 1, ..., s and moreover $\gamma_i = \tilde{\gamma}_i, \, \tilde{\delta}_i = \delta_i, \, d_i = \tilde{d}_i$ and $e_i = \tilde{e}_i$ for all i = 1, ..., s. Now, by (3.4) we have

$$\sum_{i=1}^{s} \omega_i \gamma_i^2 = \sum_{i=1}^{s} \frac{(\omega_i - d_i)^2}{\omega_i} = \sum_{i=1}^{s} (\omega_i - 2d_i + \frac{d_i^2}{\omega_i}) = \frac{1}{3}$$
(3.5)

and similarly,

$$\sum_{i=1}^{s} \omega_i \, \delta_i^2 = \frac{1}{3} \qquad \text{and} \qquad \sum_{i=1}^{s} \omega_i \, \gamma_i \, \delta_i = \frac{1}{3} \,.$$

Furthermore, the third order conditions for (2.3) imply

,

$$\sum_{i=1}^{s} \omega_i c_i \gamma_i = \sum_{i=1}^{s} \omega_i c_i \left(\sum_{j=1}^{s} (\omega_j - \frac{\omega_j}{\omega_i} \tilde{a}_{ji}) \right) = \frac{1}{2} - \sum_{i=1}^{s} \sum_{j=1}^{s} \omega_j \tilde{a}_{ji} c_i = \frac{1}{3}$$

and similarly

$$\sum_{i=1}^{s} \omega_i \tilde{c}_i \gamma_i = \frac{1}{3}, \qquad \sum_{i=1}^{s} \omega_i \tilde{c}_i \delta_i = \frac{1}{3} \qquad \text{and} \qquad \sum_{i=1}^{s} \omega_i c_i \delta_i = \frac{1}{3}.$$

Therefore, it also holds

$$\sum_{i,j} \omega_i \beta_{ij} \gamma_j = \sum_{i,j} \omega_i \left(\omega_j - \frac{\omega_j}{\omega_i} a_{ji} \right) \gamma_j = \frac{1}{2} - \sum_{j=1}^s \omega_j \gamma_j \sum_{i=1}^s a_{ji} = \frac{1}{2} - \sum_{j=1}^s \omega_j \gamma_j c_j = \frac{1}{6}$$

and

$$\sum_{i,j} \omega_i \beta_{ij} \delta_j = \frac{1}{6}, \qquad \sum_{i,j} \omega_i \alpha_{ij} \gamma_j = \frac{1}{6} \qquad \text{and} \qquad \sum_{i,j} \omega_i \alpha_{ij} \delta_j = \frac{1}{6}$$

For the corresponding coupling conditions we get

$$\sum_{i,j} \omega_i \beta_{ij} c_j = \sum_{i,j} \omega_i \left(\omega_j - \frac{\omega_j}{\omega_i} a_{ji} \right) c_j = \frac{1}{2} - \sum_{j=1}^s \omega_j c_j \sum_{i=1}^s a_{ji} = \frac{1}{2} - \sum_{j=1}^s \omega_j c_j^2 = \frac{1}{6}$$

and

$$\sum_{i,j} \omega_i \beta_{ij} \tilde{c}_j = \frac{1}{6}, \qquad \sum_{i,j} \omega_i \alpha_{ij} c_j = \frac{1}{6} \qquad \text{and} \qquad \sum_{i,j} \omega_i \alpha_{ij} \tilde{c}_j = \frac{1}{6}.$$

Finally the second set of associated coupling conditions follows by the fact that

$$\gamma_i = 1 - \sum_{j=1}^s \frac{\omega_j \tilde{a}_{ji}}{\omega_i} = 1 - \frac{d_i}{\omega_i} \quad \text{and} \quad \delta_i = 1 - \sum_{j=1}^s \frac{\omega_j a_{ji}}{\omega_i} = 1 - \frac{e_i}{\omega_i}$$

such that

$$\sum_{i,j} \omega_i a_{ij} \gamma_j = \sum_{i,j} \omega_i a_{ij} \left(1 - \frac{d_j}{\omega_j} \right) = \frac{1}{2} - \sum_{j=1}^s \frac{d_j}{\omega_j} \sum_{i=1}^s \omega_i a_{ij} = \frac{1}{2} - \sum_{j=1}^s \frac{d_j e_j}{\omega_j} = \frac{1}{6}.$$

In analogous way we obtain

$$\sum_{i,j} \omega_i a_{ij} \delta_j = \frac{1}{6}, \qquad \sum_{i,j} \omega_i \tilde{a}_{ij} \gamma_j = \frac{1}{6} \qquad \text{and} \qquad \sum_{i,j} \omega_i \tilde{a}_{ij} \delta_j = \frac{1}{6}.$$

3.2. Symplecticity. Under appropriate conditions the equation (2.2c) can be explicitly solved and thus eliminated from the optimality system (2.2c): Assume that locally in the neighbourhood of a critical point $u \mapsto H_{uu}(y, u, p)$ is invertible along the trajectory, then by the implicit function theorem, we deduce the existence of a function $u = \varphi(y, p)$ that such that (2.2c) is satisfied [3, 6, 16]. Using the function $\varphi(y, p)$ the associated reduced Hamiltonian system is then

$$\dot{y} = \mathcal{H}_p(y, p) = f(y, \varphi(y, p)) + g(y, \varphi(y, p))$$
(3.6a)

$$\dot{p} = -\mathcal{H}_y(y, p) = -f_y(y, \varphi(y, p))^T p - g_y(y, \varphi(y, p))^T p,$$
(3.6b)

where $\mathcal{H}(y, p) := H(y, \varphi(y, p), p)$. This system is a Hamiltionian differential equation [11, 6]. It has been shown [11], that in general integration methods that preserve the geometric properties such as symplecticity are more suitable to solve Hamiltionian systems [6]. However, for optimal control problems, the advantage of symplectic integrators is not as clear, but there are cases where they provide a significant computational advantage [6].

Consider the discrete Hamiltionian system

$$\dot{y}_i = -H_{p_i}(y, p), \qquad \dot{p}_i = H_{y_i}(y, p) \qquad i = 1, ..., K$$
(3.7)

It is known that the flow ψ_t generated in the phase space $\mathbb{R}^K \times \mathbb{R}^K$ of (y, p) by the equations (3.7) is symplectic, i.e. it preserves the the differential 2-form $\omega^2 = \sum_{i=1}^{K} dy_i \wedge dp_i$. Here, the differentials dy_i and dp_i at the stage *i* are computed as derivatives of the flow with respect to the initial data. Preserving the differential 2form is equivalent [11] to $\psi_t * \omega^2 = \omega^2$ for the flow ψ_t . As an important consequence we have hat the flow is volume and orientation preserving. Numerical methods that preserve symplecticity are called symplectic. There exist a variety of papers on symplectic RK methods for example [15, 22, 21, 6].

Theorem 3.2 gives conditions such that the discretization scheme (2.3) together with (2.8) is symplectic for (3.6). We assume that u is given by $u = \varphi(y, p)$ and (2.14) is locally equivalent to $u_n^i = \tilde{\varphi}(Y_n^{(i)}, P_n^{(i)}, \tilde{P}_n^{(i)})$. Here, $\tilde{\varphi}$ is the corresponding implicitly defined function that belongs to (2.13) and we identify $\tilde{\varphi}(y, p, \tilde{p}) = \varphi(y, p)$ for all (p, \tilde{p}) with $p \equiv \tilde{p}$.

THEOREM 3.2. Assuming that (2.14) holds and provided that $\tilde{\omega}_i = \omega_i$ for all i = 1, ..., s, then the discretization scheme (2.3) together with (2.8) is a symplectic scheme for (3.6). The proof of this theorem follows along the lines of the proof of Theorem 16.6 in [11].

Proof. Consider the discretization scheme (2.3) together with (2.8) as a discretization of (3.6). Moreover, to simplify the notation replace the time indices n and n + 1 by 0 and 1, respectively and let K be the dimension of y_0 or p_0 , respectively. In order to prove the symplecticity of our discretization scheme, we need to show that

$$\sum_{r=1}^{K} dy_1^r \wedge dp_1^r = \sum_{r=1}^{K} dy_0^r \wedge dp_0^r.$$

First we simplify each summand $dy_1^r \wedge dp_1^r - dy_0^r \wedge dp_0^r$ independently. Using (5.1) (see appendix), we replace dy_1^r and dp_1^r and obtain

$$dy_{1}^{r} \wedge dp_{1}^{r} - dy_{0}^{r} \wedge dp_{0}^{r} = -h \sum_{i=1}^{s} \tilde{\omega}_{i} (dy_{0}^{r} \wedge dQ_{i}^{r}) - h \sum_{i=1}^{s} \omega_{i} (dy_{0}^{r} \wedge dV_{i}^{r})$$
(3.8a)

$$+h\sum_{i=1}^{s}\tilde{\omega}_{i}(dT_{i}^{r}\wedge dp_{0}^{r})+h\sum_{i=1}^{s}\omega_{i}(dL_{i}^{r}\wedge dp_{0}^{r})$$
(3.8b)

$$-h^2 \sum_{i,j} \tilde{\omega}_i \tilde{\omega}_j (dT_i^r \wedge dQ_j^r) - h^2 \sum_{i,j} \tilde{\omega}_i \omega_j (dT_i^r \wedge dV_j^r) (3.8c)$$

$$-h^2 \sum_{i,j} \omega_i \tilde{\omega}_j (dL_i^r \wedge dQ_j^r) - h^2 \sum_{i,j} \omega_i \omega_j (dL_i^r \wedge dV_j^r) (3.8d)$$

Next we replace dy_0^r and dp_0^r by terms resulting from (5.1) and insert the corresponding terms into (3.8), then the rhs of (3.8) simplifies to

$$dy_1^r \wedge dp_1^r - dy_0^r \wedge dp_0^r = -h \sum_{i=1}^s \tilde{\omega}_i (dY_i^r \wedge dQ_i^r) - h \sum_{i=1}^s \tilde{\omega}_i (dY_i^r \wedge dV_i^r) \quad (3.9a)$$

$$+h\sum_{i=1}^{s}\tilde{\omega}_{i}(dT_{i}^{r}\wedge d\tilde{P}_{i}^{r})+h\sum_{i=1}^{s}\tilde{\omega}_{i}(dL_{i}^{r}\wedge dP_{i}^{r})-h^{2}\sum_{i,j}M_{ij}^{1}(dT_{i}^{r}\wedge dQ_{j}^{r})$$
(3.9b)

$$-h^{2} \sum_{i,j} M_{ij}^{2} (dL_{i}^{r} \wedge dQ_{j}^{r}) - h^{2} \sum_{i,j} M_{ij}^{3} (dT_{i}^{r} \wedge dV_{j}^{r}) - h^{2} \sum_{i,j} M_{ij}^{4} (dL_{i}^{r} \wedge dV_{j}^{r}) \quad (3.9c)$$

Here, the entries of the matrices M^1, M^2, M^3 and M^4 are

$$\begin{split} M^1_{ij} &= \tilde{\omega}_i \tilde{\omega}_j - \tilde{\omega}_j \tilde{a}_{ji} - \tilde{\omega}_i \tilde{\alpha}_{ij} & M^2_{ij} &= \omega_i \tilde{\omega}_j - \tilde{\omega}_j a_{ji} - \omega_i \tilde{\beta}_{ij} \\ M^3_{ij} &= \tilde{\omega}_i \omega_j - \omega_j \tilde{a}_{ji} - \tilde{\omega}_i \alpha_{ij} & M^4_{ij} &= \omega_i \omega_j - \omega_j a_{ji} - \omega_i \beta_{ij}. \end{split}$$

Hence, using the coefficients $\tilde{\alpha}_{ij}$, α_{ij} , $\tilde{\beta}_{ij}$ and β_{ij} all entries of M^1, M^2, M^3 and M^4 vanish. Using $\tilde{\omega}_i = \omega_i$ for all i = 1, ..., s we compute

$$\begin{split} \sum_{r=1}^{K} (dy_1^r \wedge dp_1^r - dy_0^r \wedge dp_0^r) = &h\left[-\sum_{i=1}^{s} \omega_i \sum_{r=1}^{K} (dY_i^r \wedge (dQ_i^r + dV_i^r)) \right. \\ &\left. + \sum_{i=1}^{s} \omega_i \sum_{r=1}^{K} (dT_i^r \wedge d\tilde{P}_i^r) + (dL_i^r \wedge dP_i^r) \right]. \end{split}$$

By (5.2) we then obtain for the rhs of this equation

$$\begin{split} -h \sum_{i=1}^{s} \omega_{i} \left[\sum_{\ell,r=1}^{K} \left(\sum_{j} \frac{\partial}{\partial y^{r} \partial y^{\ell}} f^{j}(Y^{(i)}, u_{i}) \tilde{P}_{i}^{j} + \sum_{j} \frac{\partial}{\partial y^{r} \partial y^{\ell}} g^{j}(Y^{(i)}, u_{i}) P_{i}^{j} \right) (dY_{i}^{r} \wedge dY_{i}^{\ell}) \\ &+ \left(\frac{\partial}{\partial y^{r}} f^{\ell}(Y^{(i)}, u_{i}) (dY_{i}^{r} \wedge d\tilde{P}_{i}^{\ell}) + \frac{\partial}{\partial y^{r}} g^{\ell}(Y^{(i)}, u_{i}) (dY_{i}^{r} \wedge dP_{i}^{\ell}) \right) \right] \\ &+ h \sum_{i=1}^{s} \omega_{i} \left[\sum_{\ell,r=1}^{K} \left(\frac{\partial}{\partial y^{\ell}} f^{r}(Y^{(i)}, u_{i}) (dY_{i}^{\ell} \wedge d\tilde{P}_{i}^{r}) + \frac{\partial}{\partial y^{\ell}} g^{r}(Y^{(i)}, u_{i}) \right) (dY_{i}^{\ell} \wedge dP_{i}^{r}) \right]. \end{split}$$

Since $dY_i^r \wedge dY_i^\ell = -dY_i^\ell \wedge dY_i^r$ and $dY_i^r \wedge dY_i^r = 0$ holds for the exterior product (cf. [11]), the previous term vanishes and thus

$$\sum_{r=1}^{K} [(dy_1^r \wedge dp_1^r) - (dy_0^r \wedge dp_0^r)] = 0.$$

4. Numerical example and implementation. We consider the following problem taken from Hager [10]

$$\min \frac{1}{2} \int_0^1 (u^2 + 2x^2) dt \quad \text{subject to}$$
 (4.1)

$$\dot{x}(t) = \frac{1}{2}x(t) + u(t), \ x(0) = 1.$$
 (4.2)

The optimal solution is denoted by (u^*, x^*) where

$$u^{*}(t) = \frac{2(\exp(3t) - \exp(3))}{\exp(3t/2)(2 + \exp(3))}.$$
(4.3)

To illustrate the numerical methods we reformulate the problem as a singularly perturbed differential equation

min
$$c(1)$$
 subject to (4.4a)

$$\dot{c}(t) = \frac{1}{2}(u^2(t) + x^2(t) + 4z^2(t)), \ c(0) = 0$$
 (4.4b)

$$\dot{x}(t) = z(t) + u(t), \ x(0) = 1$$
(4.4c)

$$\dot{z}(t) = \frac{1}{\epsilon} (\frac{1}{2}x(t) - z(t)), \ z(0) = \frac{1}{2}$$
(4.4d)

for some $\epsilon > 0$. Note that, as $\epsilon \to 0$, in (4.4d) we get z(t) = x(t)/2 and thus substituting into (4.4c) we recover system (4.2). Taking

$$y = \begin{pmatrix} c \\ x \\ z \end{pmatrix}, \ f(y,u) = \begin{pmatrix} \frac{1}{2}(u^2 + x^2 + 4z^2) \\ z + u \\ 0 \end{pmatrix}, \ g(y) = \frac{1}{\epsilon} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2}x - z \end{pmatrix},$$

we obtain a system of the form (2.1) for a scalar valued control u(t). We discretize the system IMEX methods. We report on results for the second-order L-stable IMEX SSP2 scheme (5.1), the second-order globally stiffly accurate IMEX-GSA (5.2) and the third-order IMEX-SA3 (5.4) scheme. In all cases we consider an equidistant grid on [0, 1] with n = 1, ..., N gridpoints. In the following we set $u = (u_n)_{n=1}^N$ where $u_n = u(t_n)$ and similarly for x and c. In order to numerically solve the optimality conditions for (4.4) it remains to solve equations (2.3),(2.8) and (2.14). We do not present the detailed formulas but have some remarks concerning the implementation.

In view of the stiff source in g it is advantegous to solve instead of (2.3) the equivalent system (2.4). As mentioned below Lemma 2.2 the adjoint equation (2.8) has to be solved backwards in time. It is therefore advantegous to use the equivalent formulation (2.7). Note that the discretized terminal condition for the adjoint scheme is $p_N = (1, 0, 0)$. Furthermore, we assume for simplicity that the control u is the same on each stage. Then, equation (2.14) reads

$$\sum_{k=1}^{5} \tilde{\omega}_k f_u(Y_n^{(k)}, u_n) \tilde{P}_n^{(k)} + \omega_k g_u(Y_n^{(k)}, u_n) P_n^{(k)} = 0.$$
(4.5)

and

$$\tilde{P}_n^{(i)}h\tilde{\omega}_i = \tilde{\xi}_n^{(i)}, \ P_n^{(i)}h\omega_i = \xi_n^{(i)}$$

where $\tilde{\xi}$ and ξ are the solution to (2.7). The optimality system (2.3),(2.8), (2.14) is solved by a block Gauss–Seidel method: Provided we know u on all grid points we solve (2.4) to obtain the state y. Having u and y at hand we can solve (2.7) in order to obtain p and subsequently $\tilde{\xi}$ and ξ . However, for an arbitrary u equation (4.5) will not hold true. We therefore use a nonlinear root finding method F(u) = 0. We set

$$F(u) = \left\| (F_n(u))_{n=1}^N \right\|_2^2, \ F_n(u) = \sum_{k=1}^s f_u(Y_n^{(k)}, u_n) \tilde{\xi}_n^{(k)} + g_u(Y_n^{(k)}, u_n) \xi_n^{(k)}, \tag{4.6}$$

where $Y_n^{(k)}, \tilde{\xi}_n^{(k)}$ and $\xi_n^{(k)}$ are all dependent on u through (2.4) and (2.7), respectively. Since in the example g_y is independent of y we can solve the adjoint equations (2.7) more efficiently. We use the fact that

$$Y_n^i = y(t_n + \tilde{c}_i \Delta t) + O((\Delta t)^p),$$

where p is the order of the explicit part of the IMEX scheme. Hence, instead of computing at every time step in the adjoint equation the values Y_n^i for $i = 1, \ldots, s$ we interpolate the given data $(y_n)_n$ using a second-and third-order accurate interpolation, respectively.

We study the dependence of $F(u^*)$ on grid size and value of ϵ for the control u^* given by (4.3). This control is optimal only in the case of $\epsilon = 0$. In order to observe the convergence rates we compute a fine grid solution on N = 640 grid points. The corresponding states and adjoints are denoted by (c^*, x^*, z^*) and (p_1^*, p_2^*, p_3^*) , respectively. Note that due to the particular structure of the problem we always have $p_1^*(t) = 1$ and therefore we do not report this quantity in the tables below. We denote by $F^* = (F_n(u^*))$ and we not necessarily have $||F^*||_{\infty} = 0$ since the control u^* is not optimal for the problem (4.4) in case $\epsilon > 0$. As in [10] we also report the L^{∞} -error in the state x(t), and relaxation variable z(t) obtained on a finer grid. Convergence results for the IMEX–SA3 and IMEX–GSA are given in Table 5.5 and Table 5.6, respectively. We observe that the convergence properties in the state remain independent on ϵ . Since the IMEX–SA3 scheme is not stiffly accurate we loose third–order convergence in the relaxation variable z when ϵ is underresolved. Contrary, we observe second–order convergence also for small ϵ for the stiffly accurate IMEX–GSA scheme.

Further, we study the convergence behavior of the nonlinear root finding method. Initially, we set u(t) = 1 and subsequently solve F(u) = 0 using a standard blackbox root finding method of Matlab with termination tolerance 1.e - 08 on F. Even so $F((u_n)_n)$ is zero up to machine precision in the optimization procedure there remains a difference in the computed trajectory $(x_n)_n$ compared with x^* . The results for IMEX– SSP2 are given in Table 5.7. We observe that the L^2 -difference between analytical and numerically computed trajectory and control decreases with grid size.

5. Summary and conclusions. We investigated the application of IMEX Runge-Kutta methods to optimal control problems. In particulare we focused on order conditions and conditions for symplecticity. We studied the adjoint equations and established a commutative diagram for optimization and discretization. In particular cases previous results for single Runge-Kutta schemes could be recovered [3, 10]. Examples of up to third order IMEX Runge-Kutta methods are given and numerical results for a sample problem have been presented.

Appendix.

A1. Addenda on the proof of Lemma 2.1. The Lagrangian function of (2.10) is given by

$$\begin{aligned} \mathcal{L}(y,Y,p,\zeta) &= j(y_N) + p^0 \cdot (y_0 - y^0) \\ &+ \sum_{n=0}^{N-1} \left[p_{n+1}^T \left(-y_{n+1} + y_n + h \sum_{i=1}^s \tilde{\omega}_i f(Y_n^{(i)}, u_n^i) + h \sum_{i=1}^s \omega_i g(Y_n^{(i)}, u_n^i) \right) \\ &+ \sum_{i=1}^s (\zeta_n^{(i)})^T (-Y_n^{(i)} + y_n + h \sum_{j=1}^s \tilde{a}_{ij} f(Y_n^{(j)}, u_n^j) + h \sum_{j=1}^s a_{ij} g(Y_n^{(j)}, u_n^j)) \right] .\end{aligned}$$

To simplify the notation in the proof of Theorem 3.2, the time indices n and n+1 are replaced by 0 and 1, respectively, for the discrete approximations y_n and p_n and they are ommitted for the intermediate states, which are denoted by vectors $Y_i \in \mathbb{R}^K$,

 $P_i \in \mathbb{R}^K$ or $\tilde{P}_i \in \mathbb{R}^K$, respectively, with *i* being the index for the stages 1, ..., *s*. In this notation the schemes (2.3) and (2.8) read for i = 1, ..., s

$$Y_{i} = y_{0} + h \sum_{j=1}^{s} \tilde{a}_{ij} f(Y_{j}, u_{j}) + h \sum_{j=1}^{s} a_{ij} g(Y_{j}, u_{j}),$$

$$y_{1} = y_{0} + h \sum_{i=1}^{s} \tilde{\omega}_{i} f(Y_{i}, u_{i}) + h \sum_{i=1}^{s} \omega_{i} g(Y_{i}, u_{i})$$

and for $i = 1, \ldots, s$

$$\tilde{P}_{i} = p_{0} - h \sum_{j=1}^{s} \tilde{\alpha}_{ij} f_{y}(Y_{j}, u_{j})^{T} \tilde{P}_{j} - h \sum_{j=1}^{s} \alpha_{ij} g_{y}(Y_{j}, u_{j})^{T} P_{j}$$

$$P_{i} = p_{0} - h \sum_{j=1}^{s} \tilde{\beta}_{ij} f_{y}(Y_{j}, u_{j})^{T} \tilde{P}_{j} - h \sum_{j=1}^{s} \beta_{ij} g_{y}(Y_{j}, u_{j})^{T} P_{j}$$

$$p_{1} = p_{0} - h \sum_{i=1}^{s} \tilde{\omega}_{i} f_{y}(Y_{i}, u_{i})^{T} \tilde{P}_{i} - \sum_{i=1}^{s} \omega_{i} g_{y}(Y_{i}, u_{i})^{T} P_{i}.$$

The one-forms $dy_1^r: \mathbb{R}^{2K} \to \mathbb{R}$ and $dY_i^r: \mathbb{R}^{2K} \to \mathbb{R}$ used in the proof of Theorem 3.2 are defined by

$$z \mapsto \frac{\partial y_1^r}{\partial (y_0, p_0)} z$$
 and $z \mapsto \frac{\partial Y_i^r}{\partial (y_0, p_0)} z$,

respectively and similarly also dp_1^r , dP_i^r and $d\tilde{P}_i^r$, where y_1^r , p_1^r , Y_i^r , P_i^r and \tilde{P}_i^r , denote the *r*th component of the corresponding vector. By differentiation of the above equations with respect to (y_0, p_0) and using the linearity of the differential we obtain

$$\begin{split} dY_{i}^{r} &= dy_{0}^{r} + h\sum_{j=1}^{s}\tilde{a}_{ij}dT_{j}^{r} + h\sum_{j=1}^{s}a_{ij}dL_{j}^{r}, dy_{1}^{r} = dy_{0}^{r} + h\sum_{i=1}^{s}\tilde{\omega}_{i}dT_{i}^{r} + h\sum_{i=1}^{s}\omega_{i}dL_{i}^{r} \\ (5.1a) \\ d\tilde{P}_{i}^{r} &= dp_{0}^{r} - h\sum_{j=1}^{s}\tilde{\alpha}_{ij}dQ_{j}^{r} - h\sum_{j=1}^{s}\alpha_{ij}dV_{j}^{r}, dP_{i}^{r} = dp_{0}^{r} - h\sum_{j=1}^{s}\tilde{\beta}_{ij}dQ_{j}^{r} - h\sum_{j=1}^{s}\beta_{ij}dV_{j}^{r} \\ (5.1b) \\ dp_{1}^{r} &= dp_{0}^{r} + h\sum_{i=1}^{s}\tilde{\omega}_{i}dQ_{i}^{r} + h\sum_{i=1}^{s}\omega_{i}dV_{i}^{r} \\ (5.1c) \end{split}$$

for i = 1, ..., s and r = 1, ..., K, where

$$dT_i^r = \sum_{\ell=1}^K \frac{\partial}{\partial y^\ell} f^r(Y_i, u_i) dY_i^\ell, \ dL_i^r = \sum_{\ell=1}^K \frac{\partial}{\partial y^\ell} g^r(Y_i, u_i) dY_i^\ell,$$
(5.2a)

$$dQ_i^r = \sum_{j=1}^K \sum_{\ell=1}^K \frac{\partial^2}{\partial y^\ell \partial y^r} f^j(Y_i, u_i) \tilde{P}_i^j, \ dY_i^\ell + \sum_{j=1}^K \frac{\partial}{\partial y^r} f^j(Y_i, u_i) d\tilde{P}_i^j,$$
(5.2b)

$$dV_i^r = \sum_{j=1}^K \sum_{\ell=1}^K \frac{\partial^2}{\partial y^\ell \partial y^r} g^j(Y_i, u_i) P_i^j, \ dY_i^\ell + \sum_{j=1}^K \frac{\partial}{\partial y^r} g^j(Y_i, u_i) dP_i^j.$$
(5.2c)

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A2. Examples of IMEX schemes. We use the following convention for the names of the schemes: Name (k, σ_E, σ_I) where k is the order, σ_E the number of levels in the explicit scheme and σ_I the number of levels in the implicit scheme.

A two stage second order IMEX method, where the implicit part is L-stable, is given by Pareschi and Russo in [19]. Since $\tilde{\omega} = \omega$ the second order conditions for the

IMEX-SSP2(2,2,2) is a second-order IMEX scheme. The factor γ is given by $\gamma = 1 - 1/\sqrt{2}$.

additive RK scheme are directly satisfied. To avoid loss of accuracy in stiff problems, in order to compute a globally stiffly accurate method ($\tilde{a}_{sj} = \tilde{\omega}_j$ and $a_{sj} = \omega_j$, $j = 1, \ldots, s$ see [5]), we are forced to take $\tilde{\omega} \neq \omega$, $\tilde{\omega}_{\nu} = 0$ and impose the additional second order conditions (3.2). In this case at least 4 levels are required. An example is IMEX-GSA(2, 3, 4) reported below

IMEX-GSA(2,3,4) is a second order globally stiffly accurate scheme.

Moreover, it can be shown that for $\tilde{\omega} = \omega$ no three stages IMEX–RK that satisfies the additional third-order conditions in Theorem 3.1 with A-stable implicit integrator exist. Here, we report three stage third order IMEX–RK method such that the explicit scheme corresponds to the third-order scheme given in [10].

IMEX-HAG(3,3,3) is a third-order IMEX scheme, where $(\tilde{A}, \tilde{\omega})$ corresponds to the third-order scheme given by Hager in [10].

Finally we present a third order scheme which uses 4 levels in order to achieve better stability properties in the implicit integrator.

Note that all IMEX schemes of type ARS have $\omega_1 = 0$, such that they do not satisfy the condition $\tilde{\omega} \neq 0$ and $\omega \neq 0$. However if they are of the particular structure of [1] with $\omega_j \neq 0$ for $j \neq 1$ and $\tilde{\omega} \neq 0$, then we can still find a variable transformation such that the conclusion of Proposition 2.1 holds (see Remark in Section 2).

IMEX-SA(3, 4, 4) is a four stages, third order IMEX scheme.

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| ę | N | $ F_n(u^*) - F_n(u_n) _{\infty}$ | $ x^* - (x_n)_n _{\infty} \text{ (Ratio)} $ | $ z^* - (z_n)_n _{\infty}$ (Ratio) | $\ p_2^* - (p_{2,n})_n\ _{\infty}$ (Ratio) | $\ p_3^* - (p_{3,n})_n\ _{\infty}$ (Ratio) |
|-------|-----|------------------------------------|---|--------------------------------------|--|--|
| 1e+01 | 10 | 9.1756e-02(0.00) | 3.1890e-05(0.00) | 2.0043e-06(0.00) | 1.2265e-05(0.00) | 3.4885e-05(0.00) |
| 1e+01 | 20 | 4.5186e-02(2.03) | 3.2932e-06(9.68) | 2.0679e-07(9.69) | 1.3011e-06(9.43) | 3.6568e-06 (9.54) |
| 1e+01 | 40 | 2.1851e-02 (2.07) | 3.7927e-07 (8.68) | 2.3698e-08(8.73) | 1.4989e-07 (8.68) | 4.1983e-07 (8.71) |
| 1e+01 | 80 | 1.0192e-02(2.14) | 4.5576e-08 (8.32) | 2.8387e-09 (8.35) | 1.8000e-08 (8.33) | 5.0267e-08 (8.35) |
| 1e+01 | 160 | 4.3665e-03 (2.33) | 5.5187e-09 (8.26) | 3.4314e-10 (8.27) | 2.1781e-09 (8.26) | 6.0731e-09 (8.28) |
| 1e+01 | 320 | 1.4553e-03 (3.00) | 6.0801e-10 (9.08) | 3.7774e-11 (9.08) | 2.3984e-10 (9.08) | 6.6831 - 10 (9.09) |
| 1e+00 | 10 | 6.0739e-02(0.00) | 7.1856e-05(0.00) | 1.1252e-05(0.00) | 1.8045e-04 (0.00) | 3.6940e-04 (0.00) |
| 1e+00 | 20 | 2.9807e-02(2.04) | 7.5380e-06(9.53) | 1.3389e-06(8.40) | 2.0218e-05 (8.93) | 4.2999e-05(8.59) |
| 1e+00 | 40 | 1.4394e-02(2.07) | 8.6958e-07 (8.67) | 1.6324e-07 (8.20) | 2.3966e-06 (8.44) | 5.1837e-06 (8.30) |
| 1e+00 | 80 | 6.7095e-03 (2.15) | 1.0444e-07 (8.33) | 2.0088e-08 (8.13) | 2.9141e-07 (8.22) | 6.3527e-07 (8.16) |
| 1e+00 | 160 | 2.8737e-03 (2.33) | 1.2639e-08 (8.26) | 2.4586e-09 (8.17) | 3.5473e-08 (8.22) | 7.7621e-08 (8.18) |
| 1e+00 | 320 | 9.5761e-04 (3.00) | 1.3919e-09(9.08) | 2.7217e-10(9.03) | 3.9175e-09(9.05) | 8.5874e-09 (9.04) |
| 1e-01 | 10 | 1.2860e-02 (0.00) | 1.886e-04 (0.00) | 1.5712e-03(0.00) | 2.4410e-03(0.00) | 5.226e-03 (0.00) |
| 1e-01 | 20 | 6.2772e-03 (2.05) | 2.6021e-05 (7.26) | 2.2140e-04 (7.10) | 3.8175e-04 (6.39) | 8.2394e-04 (6.34) |
| 1e-01 | 40 | 3.0272e-03(2.07) | 3.6994e-06 (7.03) | 3.2117e-05(6.89) | 5.6588e-05 (6.75) | 1.1973e-04 (6.88) |
| 1e-01 | 80 | 1.4106e-03 (2.15) | 5.0436e-07 (7.33) | 4.4293e-06 (7.25) | 7.8629e-06 (7.20) | 1.6467e-05 (7.27) |
| 1e-01 | 160 | 6.0415e-04 (2.33) | 6.5544e-08 (7.69) | 5.7612e-07 (7.69) | 1.0298e-06 (7.64) | 2.1441e-06 (7.68) |
| 1e-01 | 320 | 2.0132e-04 (3.00) | 7.4775e-09 (8.77) | 6.5816e-08 (8.75) | 1.1802e-07 (8.73) | 2.4499e-07 (8.75) |
| 1e-04 | 10 | 7.1929e-05(0.00) | 8.6575e-05(0.00) | 8.7328e-05 (0.00) | 6.3322e-03(0.00) | 1.2066e-02(0.00) |
| 1e-04 | 20 | 1.0419e-05(6.90) | 9.0398e-06(9.58) | 4.3047e-05(2.03) | 1.3610e-03 (4.65) | 2.6616e-03 (4.53) |
| 1e-04 | 40 | 3.7855e-06(2.75) | 1.0419e-06 (8.68) | 4.8027e-05(0.90) | 3.1411e-04 (4.33) | 6.2276e-04 (4.27) |
| 1e-04 | 80 | 1.6983e-06 (2.23) | 1.2524e-07 (8.32) | 5.0930e-05(0.94) | 7.7166e-05 (4.07) | 1.5282e-04 (4.08) |
| 1e-04 | 160 | 7.2403e-07 (2.35) | 1.5191e-08 (8.24) | $5.8513e-05\ (0.87)$ | 6.1901e-05 (1.25) | 1.2381e-04 (1.23) |
| 1e-04 | 320 | 2.4114e-07 (3.00) | 7.1227e-09 (2.13) | 7.0310e-05(0.83) | 7.0572e-05 (0.88) | 1.4115e-04 (0.88) |
| * | | | | TABLE 5.5 | TABLE 5.5 | |

 u^* is given by equation (4.3) and computed on a fine grid of N = 640. The corrresponding state are (c^*, x^*, z^*) . The state $(c_n, x_n, z_n)_n$ is the discrete solution to (2.3) using u_n given by equation (4.3) on the corresponding grid N. The values of F for u^* and u_n are given by (4.6) on the respective grids where the adjoint states are obtained through (2.8) using IMEX-SA3. The value in the brackets is the residual of the current divided by the residual of the previous result.

| result. | the adjoint states are obtained through (2.8) using IMEX-GSA. The value in the brackets is the residual of the currer | solution to (2.3) using u_n given by equation (4.3) on the corresponding grid N. The values of F for u^* and u_n are giv | u^* is given by equation (4.3) and computed on a fine grid of $N = 640$. The corrresponding state are (c^*, x^*, z^*) |
|---------|---|--|--|
| | is the residual of the current divided by the residual of the previous | s of F for u^* and u_n are given by (4.6) on the respective grids where | ponding state are (c^*, x^*, z^*) . The state $(c_n, x_n, z_n)_n$ is the discrete |

| 1e-08 | 1e-08 | 1e-08 | 1e-08 | 1e-08 | 1e-08 | 1e-04 | 1e-04 | 1e-04 | 1e-04 | 1e-04 | 1e-04 | 1e-01 | 1e-01 | 1e-01 | 1e-01 | 1e-01 | 1e-01 | 1e+00 | 1e+00 | 1e+00 | 1e+00 | 1e+00 | 1e+00 | 1e+01 | 1e+01 | 1e+01 | 1e+01 | 1e+01 | 1e+01 |
|----------------------|-------------------|-------------------|-------------------|--------------------|-------------------|-------------------|-------------------|-------------------|-----------------------|-----------------------|-------------------|-------------------|-------------------|--------------------|-------------------|-------------------|--------------------|-------------------|-------------------|-------------------|--------------------|-------------------|-------------------|-------------------|--------------------|-------------------|-------------------|-------------------|-------------------|
| - | | | | | | | | | | | | | | - | · | - | | | | | | | | | | · | | | · |
| 320 | 160 | 08 | 40 | 20 | 10 | 320 | 160 | 08 | 40 | 20 | 10 | 320 | 160 | 08 | 40 | 20 | 10 | 320 | 160 | 08 | 40 | 20 | 10 | 320 | 160 | 08 | 40 | 20 | 10 |
| 5.9391e-08 (9.04) | 5.3710e-07 (8.20) | 4.4018e-06(8.18) | 3.6025e-05(8.35) | 3.0072e-04 (8.71) | 2.6200e-03(0.00) | 2.4145e-07(4.40) | 1.0622e-06(5.25) | 5.5770e-06 (6.88) | 3.8390e-05(7.95) | 3.0503e-04 (8.61) | 2.6263e-03(0.00) | 2.0138e-04(3.00) | 6.0473e-04 (2.34) | 1.4151e-03 (2.16) | 3.0602e-03 (2.13) | 6.5111e-03 (2.24) | 1.4564e-02(0.00) | 9.5763e-04(3.00) | 2.8739e-03 (2.34) | 6.7107e-03(2.15) | 1.4404e-02(2.08) | 2.9890e-02 (2.06) | 6.1450e-02(0.00) | 1.4553e-03 (3.00) | 4.3667 e-03 (2.33) | 1.0193e-02(2.14) | 2.1859e-02(2.07) | 4.5250e-02(2.04) | 9.2301e-02(0.00) |
| 4.5577e-06(5.02) | 2.2882e-05 (4.24) | 9.6931e-05 (4.12) | 3.9927e-04 (4.16) | 1.6597 e-03 (4.30) | 7.1442e-03 (0.00) | 5.1861e-06 (4.60) | 2.3832e-05 (4.10) | 9.7706e-05 (4.09) | 3.9915e-04 (4.15) | 1.6575e-03 (4.31) | 7.1375e-03 (0.00) | 7.8573e-07 (3.50) | 2.7495e-06 (4.96) | 1.3647 e-05 (6.26) | 8.5496e-05(6.43) | 5.4949e-04 (6.37) | 3.5004 e-03 (0.00) | 1.6021e-06 (4.84) | 7.7608e-06 (4.25) | 3.2950e-05(4.14) | 1.3654 e-04 (4.21) | 5.7481e-04 (4.43) | 2.5447e-03(0.00) | 1.3305e-06 (4.27) | 5.6848e-06(4.11) | 2.3345e-05(4.10) | 9.5630e-05 (4.17) | 3.9831e-04 (4.33) | 1.7243e-03 (0.00) |
| 2.2788e-06(5.02) | 1.1441e-05 (4.24) | 4.8466e-05(4.12) | 1.9964e-04 (4.16) | 8.2987e-04 (4.30) | 3.5721e-03(0.00) | 1.4779e-05(1.19) | 1.7548e-05(3.04) | 5.3299e-05(3.84) | 2.0443e-04 (4.08) | 8.3367e-04 (4.29) | 3.5731e-03(0.00) | 1.8843e-06 (4.90) | 9.2319e-06(3.97) | 3.6618e-05(3.89) | 1.4232e-04 (4.38) | 6.2277e-04 (4.55) | 2.8345 e-03 (0.00) | 8.9805e-07(5.02) | 4.5075e-06 (4.23) | 1.9085e-05(4.11) | 7.8532e-05(4.15) | 3.2585e-04 (4.29) | 1.3985e-03(0.00) | 1.3445e-07(5.02) | 6.7536e-07 (4.24) | 2.8640e-06(4.13) | 1.1824e-05(4.18) | 4.9394e-05 (4.35) | 2.1503e-04(0.00) |
| 6.4837e-06(5.01) | 3.2501e-05 (4.23) | 1.3746e-04 (4.11) | 5.6437e-04 (4.13) | 2.3297e-03 (4.24) | 9.8738e-03(0.00) | 2.6513e-05 (2.46) | 6.5098e-05 (2.71) | 1.7626e-04 (3.43) | 6.0419e-04 (3.91) | 2.3649e-03 (4.18) | 9.8943e-03(0.00) | 1.5388e-05 (4.91) | 7.5515e-05 (4.05) | 3.0554e-04 (3.78) | 1.1543e-03 (3.57) | 4.1263e-03(3.40) | 1.4019e-02(0.00) | 1.3160e-06(4.41) | 5.8078e-06(4.03) | 2.3378e-05 (4.04) | 9.4343e-05 (4.10) | 3.8663e-04 (4.20) | 1.6246e-03(0.00) | 2.9758e-07(5.03) | 1.4979e-06 (4.26) | 6.3807e-06(4.17) | 2.6590e-05 (4.26) | 1.1331e-04 (4.55) | 5.1541e-04 (0.00) |
| 4.1090e-11(3.06) | 1.2566e-10 (2.38) | 2.9937e-10 (2.21) | 6.6291e-10 (2.20) | 1.4556e-09 (2.28) | 3.3238e-09(0.00) | 5.3256e-05 (1.64) | 8.7494e-05(1.21) | 1.0612e-04 (1.07) | $1.1350e-04 \ (0.98)$ | $1.1131e-04 \ (0.86)$ | 9.5557e-05 (0.00) | 2.7456e-05 (4.89) | 1.3418e-04 (4.01) | 5.3793e-04 (3.70) | 1.9908e-03 (3.41) | 6.7796e-03 (3.01) | 2.0384e-02(0.00) | 3.4393e-07(5.00) | 1.7202e-06 (4.20) | 7.2297e-06 (4.05) | 2.9295e-05 (4.02) | 1.1769e-04 (4.01) | 4.7224e-04 (0.00) | 4.9649e-07 (5.00) | 2.4821e-06 (4.20) | 1.0420e-05 (4.04) | 4.2111e-05(3.99) | 1.6797e-04 (3.91) | 6.5622e-04 (0.00) |

| N | ϵ | $ F_n(u_n)_n _2^2$ | $\ x^* - (x_n)_n\ _{\infty}$ | $\ u^* - (u_n)_n\ _{\infty}$ |
|-----|------------|----------------------|------------------------------|------------------------------|
| 10 | 0e + 00 | 9.3435e-16 | 1.1661e-01 (0.00) | 8.1212e-02(0.00) |
| 20 | 0e + 00 | 5.7291e-15 | 5.4444e-02(2.14) | 3.5548e-02(2.28) |
| 40 | 0e + 00 | 2.1384e-14 | 2.5674e-02(2.12) | 1.6495e-02(2.16) |
| 80 | 0e + 00 | 4.8134e-13 | 1.1822e-02(2.17) | 7.9952e-03(2.06) |
| 160 | 0e + 00 | 5.2921e-13 | 5.0243e-03(2.35) | 3.7065e-03(2.16) |
| 320 | 0e + 00 | 4.9687e-11 | 1.6345e-03(3.07) | 1.4217e-03(2.61) |
| 10 | 1e-02 | 9.2474e-16 | 1.1649e-01(0.00) | 8.0766e-02(0.00) |
| 20 | 1e-02 | 4.6022e-15 | 5.4428e-02(2.14) | 3.5485e-02(2.28) |
| 40 | 1e-02 | 1.6138e-13 | 2.5673e-02(2.12) | 1.6428e-02(2.16) |
| 80 | 1e-02 | 4.0505e-13 | 1.1818e-02(2.17) | 7.9385e-03(2.07) |
| 160 | 1e-02 | 4.9368e-13 | 5.0148e-03 (2.36) | 3.6611e-03(2.17) |
| 320 | 1e-02 | 2.1669e-11 | 1.6241e-03 (3.09) | 1.4336e-03 (2.55) |
| 10 | 1e-01 | 8.7718e-15 | 1.1655e-01 (0.00) | 7.9657e-02(0.00) |
| 20 | 1e-01 | 6.4816e-15 | 5.4631e-02(2.13) | 3.5508e-02(2.24) |
| 40 | 1e-01 | 2.9944e-14 | 2.5813e-02(2.12) | 1.6218e-02(2.19) |
| 80 | 1e-01 | 5.3096e-14 | 1.1900e-02(2.17) | 7.6948e-03(2.11) |
| 160 | 1e-01 | 1.0236e-13 | 5.0614e-03 (2.35) | 3.4365e-03(2.24) |
| 320 | 1e-01 | 4.4261e-11 | 1.6702e-03(3.03) | 1.1434e-03(3.01) |
| 10 | 1e + 00 | 3.6848e-15 | 1.0539e-01(0.00) | 6.7925e-02(0.00) |
| 20 | 1e + 00 | 9.3571e-16 | 4.9678e-02(2.12) | 3.0924e-02(2.20) |
| 40 | 1e + 00 | 3.8451e-16 | 2.3511e-02(2.11) | 1.4248e-02(2.17) |
| 80 | 1e + 00 | 2.5252e-13 | 1.0821e-02(2.17) | 6.3999e-03 (2.23) |
| 160 | 1e + 00 | 3.9397e-12 | 4.5746e-03 (2.37) | 2.5857e-03 (2.48) |
| 320 | 1e + 00 | 1.9792e-12 | 1.4744e-03 (3.10) | 7.3745e-04(3.51) |
| | | | TABLE 5.7 | |

 u^* is the numerically obtained control (4.3) on a grid with N = 640 mesh points after computation of $F(u^*) = 0$. with initial value u(t) = 1 for the Gauss-Seidel iteration. $(u_n)_n$ is the numerically obtained control after succesful computation of F(u) = 0 with the same initial value for the Gauss-Seidel iteration. The corresponding states are x^* and $(x_n)_n$, respectively, and they are the discrete solution to (2.3). Note that in order to compute $F((u_n)_n)$ the adjoint states have obtained through (2.8) using IMEX SSP2. The value in the brackets is the residual of the current divided by the residual of the previous result.