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Abstract. We are interested in a class of numerical schemes for the optimization of nonlinear hyperbolic partial differential equations. We present continuous and discretized relaxation schemes for scalar, one–conservation laws. We present numerical results on tracking type problems with nonsmooth desired states and convergence results for higher–order spatial and temporal discretization schemes.

Keywords: IMEX schemes, optimal control, conservation laws, Runge-Kutta methods

1 Introduction

We consider an optimal control problem for scalar conservation laws of the type

$$\begin{aligned} &\text{minimize}_{u_0} \ J(u(T), u_0) \\ &\text{subject to } u_t + f(u)_x = 0, \qquad u(0, x) = u_0(x), \end{aligned} \tag{1}$$

Here, J and f are assumed to be smooth and possibly nonlinear functions. The initial value u_0 acts as control to the problem. It can be observed that the wave interactions that occur in the solution u in the case of a nonlinear flux function f pose the serious analytical challenges. Recently, the differentiability of J with respect to u_0 could be proven in the sense of shift–differentiability. We refer to [6, 9–11, 28–30, 4, 32] for more details.

Here, a class of numerical methods applied to the optimal control problem (1) is studied. We only consider the case of smooth initial data and smooth solutions u and refer to [4] for more details. For a numerical analysis including shock waves and in the case of the Lax–Friedrichs scheme we refer to [21, 32] and the references therein.

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1.1   Relaxation Method

As motiviation for a numerical scheme we follow the ideas of Jin and Xin [22]. Therein, a linear approximation (2) of the nonlinear hyperbolic equation

$$\partial_t u + \partial_x f(u) = 0$$

has been discussed. For initial conditions $u(x,0) = u_0$ the approximation is

$$\begin{aligned}
\partial_t u + \partial_x v &= 0\,, & u(x,0) &= u_0, \\
\partial_t v + a^2 \partial_x u &= \tfrac{1}{\epsilon}\left(f(u) - v\right)\,, & v(x,0) &= f(u_0)
\end{aligned} \tag{2}$$

where $\varepsilon > 0$ is the relaxation rate and a is a given constant satisfying the subcharacteristic condition $\max_u |f'(u)| \le a$. For ε being small, the solution u of (2) satisfies $\partial_t u + \partial_x f(u) = \varepsilon \partial_x((a^2 - f(u)^2)\partial_x u)$ (cf. [22]). Applying the relaxation to the optimal control problem (1), we obtain

$$\min_{u_0} J(u(\cdot, T), u_0) \quad \text{subject to} \quad
\begin{cases}
u_t + v_x = 0, \\
v_t + a^2 u_x = \tfrac{1}{\epsilon}\left(f(u) - v\right), \\
u(0,x) = u_0, \ v(0,x) = f(u_0)
\end{cases} \tag{3}$$

The corresponding adjoint equations for (3) are given by (cf. [?])

$$-p_t - a^2 q_x = \frac{q}{\epsilon} f'(u), \quad p(T,x) = p_T(x),$$

$$-q_t - p_x = -\frac{q}{\epsilon}, \quad q(T,x) = q_T(x).$$

For more information on the relaxation system, its limiting scheme for $\epsilon = 0$, further numerical analysis and extensions we refer to $[1, 2, 5, 14, 3, 8, 22, 25, 27]$ and the references therein. Also, the computations are valid provided that all appearing functions are at least once differentiable. This is in general not the case for conservation laws.

2   IMEX-Runge-Kutta Discretization

Numerical discretization of the relaxation system using higher order temporal discretizations combined with higher order spatial discretization has been investigated in several recent publications as for example $[22, 27]$. We apply so called implicit–explicit Runge-Kutta methods $[26, 27, 3]$ as temporal discretization (IMEX RK). Here, the expliciti integration is used for the linear hyperbolic transport part and an implicit method is applied to the the stiff source term. Implicit-explicit Runge-Kutta method have been studied in the context of control problems for example in $[4, 19]$. Define

$$\mathbf{y} = (u, v)^T, \qquad g(\mathbf{y}) = (v, a^2 u)^T \qquad \text{and} \qquad r(\mathbf{y}) := (0, -(v - f(u)))^T$$

then (2) becomes

$$\mathbf{y}_t + g(\mathbf{y})_x = \frac{1}{\varepsilon} r(\mathbf{y}), \qquad \text{and} \qquad \mathbf{y}(0, x) = (u^0, f(u^0))^T(x)$$

Applying a suitable discretization D_x of the spatial derivative yields the semi-discrete state equations

$$\mathbf{y}' = -D_x \, g(\mathbf{y}) + \frac{1}{\epsilon} r(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}^0. \tag{4}$$

Remark 1. Spatial discretizations for the linear transport part are well–known. The simplest possible is a first–order Upwind method:

$$\frac{\partial}{\partial t} \mathbf{y}_j = -\frac{1}{\Delta x} \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} (\mathbf{y}_{j+1/2} - \mathbf{y}_{j-1/2}) + \frac{1}{\epsilon} r(\mathbf{y}_j),$$

where $\mathbf{y}_{j+1/2}$ is obtained by applying the first-order upwind method to characteristic variables $v \pm au$. Higher order MUSCL schemes, WENO schemes or central schemes have also been studied in this context.

The resulting semi–discrete optimal control problem is then given by:

$$\begin{aligned} \text{minimize} \quad & j(\mathbf{y}(T), \mathbf{y}^0) \\ \text{subject to} \quad & \mathbf{y}' = -D_x \, g(\mathbf{y}) + \tfrac{1}{\epsilon} r(\mathbf{y}), \qquad \mathbf{y}(0) = \mathbf{y}^0. \quad t \in [0, T] \end{aligned} \tag{5}$$

In the context of relaxation schemes the semi–discrete problem is seen as a time–integration problem with stiff source which is discretized by an IMEX RK methods. For the numerical discretization we therefore consider the previous problem as an optimal control problem involving ordinary differential equations. Literature concerning the numerical analysis of Runge-Kutta methods for the optimality system of (5) have been studied in [17, 7, 24]. In [7, 17] partitioned Runge-Kutta methods for the optimality system are obtained using the *discretize–then–optimize* approach. The derived partitioned Runge–Kutta methods have been analysed with regard to symplecticity and order of convergence. In [19], Herty and Schleper, moreover, analysed the associated adjoint imex Runge-Kutta method that one obtains if an explicit method is applied to $D_x g(y)$ and a (diagonally) implicit method to $\frac{1}{\epsilon} r(y)$. In the following, we will analyse general partitioned Runge-Kutta methods using IMEX RK methds. More details can be found in [20]. Therein, the following IMEX Runge-Kutta discretization of (4) is studied.

$$\begin{aligned} Y_n^{(i)} &= y_n + h \sum_{j=1}^{i-1} \tilde{a}_{ij} D_x g(Y_n^{(j)}) + h \sum_{j=1}^{i} a_{ij} \frac{1}{\epsilon} r(Y_n^{(j)}) & i &= 1, .., s \\ y_{n+1} &= y_n + h \sum_{i=1}^{s} \tilde{\omega}_i D_x g(Y_n^{(i)}) + h \sum_{i=1}^{s} \omega_i \frac{1}{\epsilon} r(Y_n^{(i)}), & n &= 0, 1, 2, . \end{aligned} \tag{6}$$

A nonlinear variable transformation and two intermediate states $\tilde{K}_n^{(i)}$ and $K_n^{(i)}$ give the equivalent system

$$
\begin{aligned}
\tilde{K}_n^{(i)} &= D_x g\left(y_n + h\sum_{j=1}^s \tilde{a}_{ij}\tilde{K}_n^{(j)} + h\sum_{j=1}^s a_{ij}K_n^{(j)}\right) & i = 1,..,s \\
K_n^{(i)} &= \frac{1}{\epsilon} r\left(y_n + h\sum_{j=1}^s \tilde{a}_{ij}\tilde{K}_n^{(j)} + h\sum_{j=1}^s a_{ij}K_n^{(j)}\right) & i = 1,..,s \\
y_{n+1} &= y_n + h\sum_{i=1}^s \tilde{\omega}_i \tilde{K}_n^{(i)} + h\sum_{i=1}^s \omega_i K_n^{(i)}, & n = 0,1,2,.
\end{aligned}
\tag{7}
$$

The associated optimality systems for the two previous optimization problems then coincide and we refer to [20] for mor details. It is proven that the adjoint schemes are equivalent to

$$
\tilde{P}^{(i)} = p_n - h\sum_{j=1}^s \tilde{\alpha}_{ij}\, g'(Y_n^{(j)})^T \bar{D}_x \tilde{P}^{(j)} - h\sum_{j=1}^s \alpha_{ij}\frac{1}{\epsilon}r'(Y_n^{(j)})^T P^{(j)} \qquad i = 1,..,s
$$

$$
P^{(i)} = p_n - h\sum_{j=1}^s \tilde{\beta}_{ij}\, g'(Y_n^{(j)})^T \bar{D}_x \tilde{P}^{(j)} - h\sum_{j=1}^s \beta_{ij}\frac{1}{\epsilon}r'(Y_n^{(j)})^T P^{(j)} \qquad i = 1,..,s \tag{8}
$$

$$
p_{n+1} = p_n - h\sum_{i=1}^s \tilde{\omega}_i g'(Y_n^{(i)})^T \bar{D}_x \tilde{P}^{(i)} - h\sum_{i=1}^s \omega_i \frac{1}{\epsilon}r'(Y_n^{(i)})^T P^{(i)} \qquad n = 0,1,..,N-1
$$

Here, the coefficients of the Runge-Kutta method $\tilde{\alpha}_{ij}, \alpha_{ij}, \tilde{\beta}_{ij}$ and β_{ij} are given by

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

2.1   Properties of Discrete IMEX-RK Optimality System

For the resulting scheme (6),(8) order conditions can be stated [20]. To this end we add a suitable equation for $\tilde{p}$ to the previous system.

$$
\tilde{p}_{n+1} = \tilde{p}_n - h\sum_{i=1}^s \tilde{\omega}_i\, f_y(Y_n^{(i)})^T \tilde{P}^{(i)} - h\sum_{i=1}^s \omega_i\, g_y(Y_n^{(i)})^T P^{(i)}. \tag{9}
$$

The full method therefore is a standard additive Runge-Kutta scheme for

$$
\mathbf{y}' = -D_x\, g(\mathbf{y}) + \frac{1}{\epsilon}r(\mathbf{y})
$$

$$
\tilde{\mathbf{p}}' = g'(\mathbf{y})^T D_x \tilde{\mathbf{p}} + \frac{1}{\epsilon}r'(\mathbf{y})^T \mathbf{p}
$$

$$
\mathbf{p}' = g'(\mathbf{y})^T D_x \tilde{\mathbf{p}} + \frac{1}{\epsilon}r'(\mathbf{y})^T \mathbf{p}
$$

If we define

$$
c_i := \sum_{j=1}^s a_{ij}, \qquad \text{and} \qquad \tilde{c}_i := \sum_{j=1}^s \tilde{a}_{ij},
$$

$$\gamma_i := \sum_{j=1}^{s} \alpha_{ij}, \qquad \text{and} \qquad \tilde{\gamma}_i := \sum_{j=1}^{s} \tilde{\alpha}_{ij},$$

$$\delta_i := \sum_{j=1}^{s} \beta_{ij}, \qquad \text{and} \qquad \tilde{\delta}_i := \sum_{j=1}^{s} \tilde{\beta}_{ij}$$

then (1) holds true.

Theorem 1. *Consider the Runge-Kutta scheme (6),(8),(9). This scheme is of*

- **First-Order** : *if (SRK1) is of first order*

- **Second-Order** : *if (SRK1) is of second order*

- **Third-Order** : *if (SRK1) is of third order and either*

$$\sum_{i=1}^{s} \omega_i \, \gamma_i^2 = \frac{1}{3}, \qquad \sum_{i=1}^{s} \omega_i \, \tilde{\gamma}_i^2 = \frac{1}{3}, \qquad \sum_{i=1}^{s} \omega_i \, \gamma_i \tilde{\gamma}_i = \frac{1}{3},$$

are satisfied or if

$$\sum_{i=1}^{s} \omega_i \, a_{ij} \, \gamma_i = \frac{1}{6}, \qquad \sum_{i=1}^{s} \omega_i \, \tilde{a}_{ij} \, \tilde{\gamma}_i = \frac{1}{6}$$

and if

$$\sum_{i=1}^{s} \omega_i \, a_{ij} \, \tilde{\gamma}_i = \frac{1}{6} \qquad \text{or} \qquad \sum_{i=1}^{s} \omega_i \, \tilde{a}_{ij} \, \gamma_i = \frac{1}{6}$$

are satisfied.

Note that the system (6) and (8) is not completely coupled, since the forward scheme (6) is solved independently of the adjoint scheme (8). General order conditions can be found e.g. in [23]. The proof of Theorem 1 and together with more details are discussed in [20].

3   Numerical Results

3.1   Scalar Example

As a simple example, we use a tracking type functional $J(u)$ together with Burgers' equation

$$u_t + \left(\frac{u^2}{2} \right)_x = 0,$$

and the desired state u_d at final time $T = 2.0$, that belongs to the initial condition $u_d(0, x) = \frac{1}{2} + \sin(x)$ and we start the optimization with the initial data

$u^s(0, x) \equiv 0.5$. Moreover, the spatial interval is given by $x \in [0, 2\pi]$, As discretization of the objective functional, we use

$$J(u(\cdot, T), u_0, u_d) = \frac{\Delta x}{2} \sum_{i=1}^{K} \|u_i - u_{d\,i}\|^2.$$

Moreover, the discrete gradient of the reduced cost functional is given by

$$\nabla_{u_{0,i}} \tilde{J} = p_{0,i} + (Df(u_0)^T \mathbf{q}_0)_i.$$

In order to solve the optimal control problem, we apply a steepest descent method (with respect to the reduced cost functional) with fixed stepsize $0 < \alpha < 1$, i.e. we set $u_0^{k+1} = u_0^k + \alpha \nabla_{u_{0,i}} \tilde{J}$. As stopping criterion for the optimization process we test $|\tilde{J}(u_0, u_d)| < tol$ where $tol = 1E - 2$ denotes a predefined stopping tolerance. We observe grid independence in the case where u and u_0 are differentiable in space and time.

As first-order scheme, we test the Implicit-Explicit Euler scheme

$$\begin{aligned} u_i^* &= u_i^n \\ v_i^* &= v_i^n - \frac{\Delta t}{\epsilon}(v_i^* - f(u_i^*)) \\ u_i^{n+1} &= u_i^* - \Delta t \, D_x v_i^* \\ v_i^{n+1} &= v_i^* - \Delta t \, a^2 D_x v_i^* \end{aligned}$$

for the forward, as well as for the backward

$$\begin{aligned} q_i^* &= q_i^{n+1} - \Delta t D_x^* p_i^{n+1} \\ p_i^* &= p_i^{n+1} - \Delta t \, a^2 D_x^* q_i^{n+1} \\ q_i^n &= q_i^* - \frac{\Delta t}{\epsilon} q_i^n \\ p_i^n &= p_i^* + \frac{\Delta t}{\epsilon} q_i^n f'(u_i^n) \end{aligned}$$

The spatial gridsize is chosen to be $N_x = 300$, whereas the time discretization is done according to the CFL condition with constant $c_{CFL} = 0.5$.
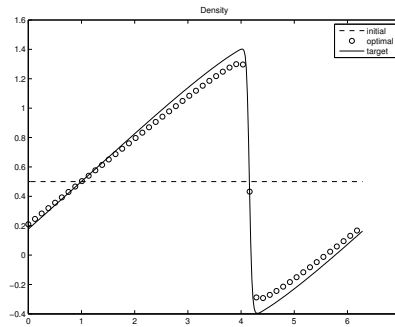
N	Nr. of It.	CPU time (in sec.)
100	44	1.795572e+01
150	43	3.768984e+01
200	42	6.380441e+01
300	41	1.491838e+02

4 Summary

We briefly discussed a class of numerical methods applied to an optimal control problem for scalar, hyperbolic partial differential equations. Order conditions for the temporal numerical discretization in the case of differentiable functions have been stated. Future work includes the analysis of additional properties of the derived numerical discretizations as for example strong stability and asymptotic preservation properties.

Acknowledgments.

Appendix.

The discrete adjoint equations that correspond to the discrete optimization problem associated with (7) are

$$\tilde{\xi}_n^{(i)} = h\,\tilde{\omega}_i\,p_{n+1} + h\sum_{j=1}^{s}\tilde{a}_{ji}g'(Y_n^{(j)})^T\bar{D}_x\tilde{\xi}_n^{(j)} + h\sum_{j=1}^{s}\tilde{a}_{ji}\frac{1}{\epsilon}r'(Y_n^{(j)})^T\xi_n^{(j)}$$

$$\xi_n^{(i)} = h\,\omega_i\,p_{n+1} + h\sum_{j=1}^{s}a_{ji}g'(Y_n^{(j)})^T\bar{D}_x\tilde{\xi}_n^{(j)} + h\sum_{j=1}^{s}a_{ji}\frac{1}{\epsilon}r'(Y_n^{(j)})^T\xi_n^{(j)}$$

$$p_n = p_{n+1} + \sum_{i=1}^{s}g'(Y_n^{(i)})^T\bar{D}_x\tilde{\xi}_n^{(i)} + \sum_{i=1}^{s}\frac{1}{\epsilon}r'(Y_n^{(i)})^T\cdot\xi_n^{(i)}$$

$$p_N = j'(y_N, y^0)\,.$$

Moreover, the variable transformation that is needed to obtain (8) is given by

$$\tilde{P}_n^{(i)} := \frac{\tilde{\xi}_n^{(i)}}{h\,\tilde{\omega}_i} \qquad \text{and} \qquad P_n^{(i)} := \frac{\xi_n^{(i)}}{h\,\omega_i} \qquad (i = 1,..,s; \quad n = 0,..,N-1)\,.$$

On the other hand, using (6) the associated discrete adjoint equations are

$$\zeta_n^{(i)} = h \left(\tilde{\omega}_i f_y(Y_n^{(i)}) + \omega_i g_y(Y_n^{(i)}) \right)^T p_{n+1} + \sum_{j=1}^{s} \tilde{a}_{ji} \, f_y(Y_n^{(i)})^T \zeta^{(j)}$$

$$+ h \sum_{j=1}^{s} a_{ji} \, g_y(Y_n^{(i)})^T \zeta^{(j)} \qquad i = 1, .., s$$

$$p_n = p_{n+1} + \sum_{i=1}^{s} \zeta_n^{(i)}, \qquad i = 1, .., N-1, \qquad p_N = j'(y_N)$$

which can be transformed into the scheme (8) using the variable transformation

$$\tilde{P}_n^{(i)} := p_{n+1} + \sum_{j=1}^{s} \frac{\tilde{a}_{ji}}{\tilde{\omega}_i} \zeta_n^{(j)} \qquad \text{and} \qquad P_n^{(i)} := p_{n+1} + \sum_{j=1}^{s} \frac{a_{ji}}{\omega_i} \zeta_n^{(j)} .$$

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