

## Numerics and Control of Conservation Laws

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Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

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## NUMERICS AND CONTROL OF CONSERVATION LAWS \*

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**Abstract.** This article aims to present a review of existing results on theoretical and numerical aspects of the control of hyperbolic balance laws. Several aspects will be covered including the differential calculus in the presence of weak entropic discontinuous solutions in the scalar and system's case as well as results on the non–conservative adjoint equations. A further focus is on suitable numerical integration methods and their convergence properties for state and adjoint equation. Results on several different numerical schemes that are mostly of finite–volume type are presented. Recent extensions up to the state–of–the–art are discussed and an extensive list of references for further reading is given.

 ${\bf Key}$  words. conservation laws, optimal control, numerical schemes, adjoint equation, convergence analysis

AMS subject classifications. 68Q25, 68R10, 68U05

1. Introduction. In this overview article we consider the numerical approximation of optimal control problems for hyperbolic conservation laws as well as systems of hyperbolic conservation laws including a possible source term. The prototypical optimal control problem that we will use for concreteness is of the form

(1.1) 
$$\min_{y,u} J(y) + R(u),$$
  
s.t.  $(y,u) \in Y_{ad} \times U_{ad}, y$  is the entropy solution of (1.2),

where the state equation is a hyperbolic balance law or a system of balance laws

(1.2) 
$$\begin{aligned} \partial_t y + \partial_x f(y) &= g \quad \text{on } \ \mathbb{R}_T \coloneqq (0,T) \times \mathbb{R} \\ y(0,\cdot) &= u \quad \text{on } \ \mathbb{R}, \end{aligned}$$

The objective functional J is assumed to be of the integral form

(1.3) 
$$J(y) := \int_{\mathbb{R}} \gamma(x)\psi(y(T,x), y_d(x)) \,\mathrm{d}x$$

for some function  $\psi \in C^{1,1}(\mathbb{R}^{2n})$  depending on a desired state of bounded variation (BV)

$$y_d \in BV_{\text{loc}}(\mathbb{R};\mathbb{R}^n) \cap L^{\infty}(\mathbb{R};\mathbb{R}^n)$$

as well as the solution  $y \in Y \subset C([0,T]; L^1_{loc}(\mathbb{R}; \mathbb{R}^n))$  at some terminal time T > 0. Due to the regularity of the solution y pointwise functionals in time are well-defined. However, the (similar case) of functionals being averaging other solution over a possibly infinite time horizon might also be considered using a similar calculus, but have so far not been investigated in detail in the literature.

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The function  $\gamma \in C_c^1(\Omega)$  is a weight function. We denote by

$$y \in Y \subset C([0,T]; L^1_{\text{loc}}(\mathbb{R}; \mathbb{R}^n))$$

the state,  $u \in U \subset L^{\infty}(\mathbb{R};\mathbb{R}^n)$  the control,  $f \in C^2(\mathbb{R}^n;\mathbb{R}^n)$  is a flux function, and  $g \in C^2(\mathbb{R}_T;\mathbb{R}^n)$  a source term.

The term R(u) is a regularization term depending on the application, for example of the form  $\frac{\kappa}{2} \|u\|_{L^2}^2$ ,  $\kappa \|u\|_{L^1}$ , or  $\kappa \|u\|_{TV}$  with a regularization parameter  $\kappa \geq 0$ . Together with the choice of  $U_{ad}$  it ensures existence of optimal solutions [84] and influences the regularity and structure of optimal controls. Since the algorithmic treatment of regularization terms in optimal control is well understood and does not pose additional difficulties for hyperbolic problems, we will only focus on the state dependent part J(y) of the objective function.

Further regularity requirements will be stated later as needed as well as possible additional regularization terms of the control. For some results we need an objective function with smoothed observation, where we choose for concreteness a convolution leading to

(1.4) 
$$J^{s}(y) := \int_{\mathbb{R}} \gamma(x)\psi((\phi * y(T))(x), \phi * y_{d}(x)) \,\mathrm{d}x$$

with a symmetric mollifier  $\phi \in C^1_c(\mathbb{R})$ . For the considered case, there has been tremendous progress in both analytical and numerical studies of sensitivities of ywith respect to initial data u that will be reviewed in detail below. Publications treating differentiability questions have been started around 1995 in order to develop a well-posedness theory for system of conservation laws. Note that, even in the scalar case without source terms, it has been shown that the evolution operator  $\mathcal{S}_t: u(\cdot) \to \mathcal{S}_t$  $y(t, \cdot) = \mathcal{S}_t u(\cdot)$  generated by the conservation law is generically non-differentiable in  $L^1$ , see e.g. [19, 54] for examples. Theoretical results on the first-order sensitivities of  $\mathcal{S}_t y$  with respect to u has been established for general, spatially one-dimensional systems of conservation laws. Here, the initial data u are assumed to be piecewise Lipschitz continuous and contain finitely many discontinuities. Therein, the concept of tangent vectors has been introduced to characterize the evolution of variations with respect to u, see [18]. Moreover, the Lipschitz continuous dependence of  $\mathcal{S}_t$  in  $L^1$  on the initial data u has been shown in [15] and an adjoint calculus as well as optimality conditions have been derived in [20]. Results on the existence of optimal controls are given in [26, 4, 3, 26, 59, 60] and will be reviewed below.

In the scalar, one-dimensional case the results were extended for piecewise  $C^1$  initial data u from directional variations to general variations of discontinuities and smooth parts, leading to Fréchet-type differentiability results of objective functionals, see [85, 22, 86, 87, 81], and a complete sensitivity and adjoint calculus has been developed for initial as well as initial-boundary value problems. The relation to the weak formulation has been discussed in [9] for the Burgers' equation. Further details will be given in the forthcoming sections.

Another differential structure, called shift-differentiability, see e.g. [12, Definition 5.1], for BV initial data based on a horizontal shift of its graph has been developed in [17] for the scalar case and in [12] for systems.

Numerical methods for the discretization of optimal control problems for hyperbolic conservation laws have been a topic of active research and will be discussed in more detail below. Here, we mention in particular [44, 45], where the state equation (1.2) has been discretized by a modified Lax-Friedrichs scheme with numerical viscosity  $O(h^{\rho})$ ,  $2/3 < \rho < 1$ , and convergence of the corresponding sensitivity scheme and adjoint scheme has been shown in the presence of shocks. Convergence results have also been obtained in [85, 79, 80] for state schemes satisfying a discrete one-sided Lipschitz condition (OSLC) with associated adjoint scheme and in [5, 57] for implicit-explicit methods. Other examples of finite volume methods and Lagrangian methods are given e.g. in [56, 55, 25]. Using a vanishing viscosity approach has been studied for the Burgers' equation in [75].

Again, further details will be discussed in the forthcoming sections.

Furthermore, we would like to stress the fact that a sensitivity framework as well as methods and results on optimal control of hyperbolic problems have a rich field of application in engineering [46, 60, 62, 70, 77]. Among others, external flows over trans- to supersonic aircraft and internal supersonic flows through nozzles or diffuser lead to strong shock waves. Given a design parameter for some objective function, the optimal choice of the design parameter leads naturally to a formulation (1.1) and will have to take into account the discontinuities introduced by the shocks. Given variations of the design parameter, the shock may or may not differently be propagating inside the region of the flow where the objective function is evaluated [62, 77, 46]. Another important class of applications involves networks of hyperbolic conservation laws modelling for example traffic flow [78, 83], water flow or supply networks [21, 38].

We conclude our introduction by mentioning also related work on feedback control for hyperbolic systems. Today, a rich literature based on a novel Lyapunov function exists [31, 33]. For sufficiently smooth solutions  $y \in H^2(\mathbb{R})$  their analysis yields exponential decay for any initial state  $u \in H^2(\mathbb{R})$  under possibly (strong) bounds on the norm of the initial data  $y_0$ . Most of the results discussed use a quasi-linear formulation of the state equation (1.2) and boundary control, see e.g. [30]. Several extensions towards e.g. stochastic dynamics [43], consistent numerical discretization [6, 42], input-to-state stabilization [11], networked systems [68, 39, 51] have been pursued enlarging the range of possible applications. Given the scope of this overview article we do not discuss those results in the following and refer to the recent books [29, 10] for further details.

2. Notation and Variational Calculus. In the following, we consider mainly the case of initial optimal control for weak entropic solutions and their numerical discretization. It is well known that in general weak solutions of (1.2) develop discontinuities (shocks) after finite time and that an entropy condition has to be imposed to select physically relevant solutions [37]. We recall that a convex function  $\eta \in C^1(\mathbb{R}^n)$ is an entropy for (1.2) if there exists a corresponding entropy flux  $q \in C^1(\mathbb{R}^n)$  satisfying  $Dq = D\eta Df$  such that the following entropy inequality holds in the distributional sense

$$\partial_t \eta(y) + \partial_x q(y) \le D\eta(y)g$$
 in  $\mathcal{D}'(\mathbb{R}_T)$ .

Here, Dq denotes the differential of q. The formation of discontinuities makes the analysis and numerical approximation of optimal control problems (1.1) challenging. In fact, this leads to the fact that the semi-group  $y(t) = S_t(u)$  generated by a nonlinear hyperbolic conservation law (1.2) is generically nondifferentiable in  $L^1$  even in the scalar one-dimensional (1-D) case (see, e.g., [19, Example 1]).

We will in some cases allow for piecewise  $C^1$  initial controls, where the smooth parts as well as the jump locations can be controlled. Results using piecewise Lipschitz initial controls [19] are also available, as an extension towards BV controls [17, 12] leading to a differentiable structure called shift-differentiability and this will be discussed in the forthcoming section. In the case of a single spatial dimension, d = 1, we follow [86] and consider initial controls of the form

(2.1) 
$$u(x) = 1_{(-\infty,x_1]}(x)u^0(x) + \sum_{j=1}^{N-1} 1_{(x_j,x_{j+1}]}(x)u^j(x) + 1_{(x_N,\infty]}(x)u^N(x), \ x \in \mathbb{R},$$

where

$$w := (u^0, \dots, u^N, x_1, \dots, x_N) \in C_c^1((a, b); \mathbb{R}^d)^{N+1} \times \mathbb{R}^N =: W$$

are the controls. Now let

$$W_{ad} = \{ (u^0, \dots, u^N, x_1, \dots, x_N) \in W : \ a < x_1 < \dots < x_N < b \}.$$

The mapping

$$w \in W_{ad} \subset W \mapsto u(\cdot; w) \in L^1(\mathbb{R})$$

is Lipschitz continuous but only differentiable in the weak\*-topology of measures. The admissible controls may be subject to further constraints as e.g. box constraints. Hence, the set  $W_{ad}$  might be a subset of W.

Let  $\mathcal{M}_{loc}(\mathbb{R})$  denote the space of locally bounded regular Borel measures. It is easy to see that

(2.2) 
$$w \in W_{ad} \subset W \mapsto (u(\cdot; w)) \in (\mathcal{M}_{loc}(\mathbb{R})\text{-weak}^*)$$

is continuously differentiable with derivative

$$(2.3) \qquad \qquad \delta w \in W \mapsto \delta u.$$

Here, the jumps are denoted by

(2.4) 
$$[u(x_j)] = u^{j+1}(x_j) - u^j(x_j)$$

and the notational convention  $x_0 := -\infty, x_{N+1} := \infty$  is used. The derivative fulfills

(2.5)

$$\int_{\mathbb{R}} \varphi(x) \,\delta u(\mathrm{d}x) = \sum_{j=0}^{N} \int_{x_j}^{x_{j+1}} \varphi(x) \delta u^j(x) \,\mathrm{d}x - \sum_{j=1}^{N} [u(x_j)] \delta x_j \varphi(x_j), \ \forall \varphi \in C_c((a,b)).$$

The corresponding sensitivities  $\delta y$  of the entropy solution y of (1.2) satisfy the sensitivity equation

(2.6) 
$$\begin{aligned} \partial_t \delta y + \partial_x (f'(y) \delta y) &= 0 \quad \text{on } \mathbb{R}_T, \\ \delta y(0, \cdot) &= \delta u \quad \text{on } \mathbb{R}, \end{aligned}$$

in an appropriate duality sense, see Definition 2.11.

In this article we focus on the sensitivity calculus as well as numerical approaches. We will not discuss existence of optimal controls  $u^* \in \operatorname{argmin} J(y[u])$ , but refer to results e.g. on networks [27, 4], on optimization of the scalar flux function f [3] or to hyperbolic biological models [26] for results in a particular setting. Results on the optimal control of 1D Riemann problems are also available, see e.g. [59, 60]. Further, results on regularized optimal control problems including state constraints are given in [81].

We also do not discuss algorithms for numerically computing  $u^*$  based on the sensitivities or adjoints derived above. The differential structure can be exploited in gradient descent type methods and we refer to [22, 48, 70] for an analysis in the case of Burgers' equation.

**2.1. Scalar Case.** Consider first the scalar case d = 1 with uniformly convex flux function, i.e.,  $f'' \ge m_{f''} > 0$ . This condition implies an Oleinik entropy condition. In [86, 87], see also [76, 81] for the case of boundary control, it was shown that at a control w, for which  $u(\cdot; w)$  satisfies a generic non-degeneracy assumption, the mapping

$$(2.7) w \in W \mapsto J(y(u(\cdot; w)))$$

is Fréchet-differentiable. In fact, by using Dafermos' theory of generalized characteristics [36] one can show the following [86, 87].

THEOREM 2.1. Consider (1.1) with initial data (2.2). Assume that  $\bar{w} \in W_{ad}$  is nondegenerated in the sense that  $y(u(\cdot; \bar{w}))$  has at time T on  $I := \operatorname{supp}(\gamma) = [l, r]$ with  $\gamma$  in (1.3) no shock generation points and finitely many nondegenerate shocks at  $z_1(\bar{w}) < \cdots < z_K(\bar{w})$  that are no shock interaction points. Then  $w \in W \mapsto$  $y(u(\cdot; \bar{w}))(T)$  is shift-differentiable at  $\bar{w}$  in the sense that in a neighborhood of  $\bar{w}$  the shock locations  $w \in W \mapsto z_i(w)$  and the functions

$$w \in W \mapsto y_i(w) \in C([z_{i-1}(\bar{w}), z_i(\bar{w})]), \quad i = 1, \dots, K+1,$$

depend continuously differentiable on w, where we set  $z_0(w) = l$ ,  $z_{K+1}(w) = r$  and  $y_i(w)$  is the continuous constant extension (if necessary) of  $y(u(\cdot;w))(T)|_{(z_{i-1}(w),z_i(w))}$  to  $[z_{i-1}(\bar{w}), z_i(\bar{w})]$ .

As a consequence, if  $y_d$  is continuous at  $z_i(\bar{w})$ , i = 1, ..., K, then the mapping (2.7) with (1.3) is continuously differentiable at  $\bar{w}$ . The same holds for the smoothed objective functional (1.4).

The previous result requires that  $y(T, \cdot; u(\cdot; \bar{w}))$  has on I = [l, r] finitely many nondegenerate shocks that are no shock interaction points. To explain this, we have to introduce generalized characteristics in the sense of Dafermos [36].

DEFINITION 2.2 (Generalized characteristics). A Lipschitz continuous curve  $x = \xi(t) \ t \in [a, b] \subset [0, T]$  is a (generalized) characteristic if the differential inclusion holds

$$\dot{\xi}(s) \in [f'(y(s,\xi(s)+)), f'(y(s,\xi(s)-))] \ a.a. \ s \in [a,b].$$

It can be shown [36] that under the one-sided Lipschitz condition (OSLC) (2.17) generalized forward characteristics through  $(t, x) \in \mathbb{R}_T$  are unique and will be denoted by

$$(2.8) s \in [t,T] \mapsto X(s;t,x).$$

However, backward characteristics are in general not unique, but through a point  $(t, x) \in \mathbb{R}_T$  a unique minimal backward characteristic and a unique maximal backward characteristic exists. They are genuine in the sense that they travel with classical characteristic speed  $f'(y(s, \xi(s)+)) = f'(y(s, \xi(s)-))$  for a.a.  $s \in [0, t]$ .

DEFINITION 2.3 (Nondegenerated shock). Let  $y(T, \cdot; u)$  have a shock at  $\bar{z}$ . Denote by  $\xi_{\mp}$  the minimal and maximal backward characteristic through (T, x), respectively, and set  $\bar{x}_{\mp} = \xi_{\mp}(0)$ . Then the shock is called nondegenerated if u is differentiable at  $\bar{x}_{-}$  and

$$\frac{d}{dx}X(t;0,x)|_{x=\bar{x}_-}\geq\beta>0, \quad \forall\, 0\leq t\leq T,$$

or  $\bar{x}_{-}$  is a rarefaction center (i.e., up-jump of u) and there is  $\delta > 0$  small enough such that all backward characteristics through  $(T, z), z \in (\bar{z} - \delta, \bar{z}]$ , meet t = 0 in  $\bar{z}$ and

$$\frac{d}{dx}X(t;s,x)|_{x=\xi_{-}(s)} \ge \beta \frac{t}{s} > 0, \quad \forall \, 0 < s < \delta, \quad s \le t \le T$$

and if an analogous condition holds for  $\bar{x}_+$ .

The nondegeneracy assumption ensures that  $y(T, \cdot; u)$  is  $C^1$  on both sides of the shock, which is a generic situation, see [36, 86].

The derivative of the objective functional J in (1.3) ensured by Theorem 2.1 admits with  $\delta u$  as in (2.3), (2.5) an adjoint representation. This requires some preparation.

We consider as in [86, 87] the case that in addition to the smooth control parts  $u^{j}$  only shock generating switching locations  $x_{j}$  can be controlled, i.e.,

(2.9) 
$$\delta x_j = 0 \quad \text{if } [u_0(x_j)] \ge 0.$$

In this case, the adjoint representation reads

(2.10) 
$$D_u J(y(u)) \cdot \delta u = \int_{\mathbb{R}} p(0, x) \delta u(\mathrm{d}x),$$

where, p is the reversible solution of the adjoint equation (see Definitions 2.4 and 2.8). The existence of solutions p is non-trivial due to the possible low regularity of y and we refer to Lemma 2.5 and 2.9 for a discussion.

(2.11) 
$$\partial_t p + f'(y)\partial_x p = 0$$
 on  $\mathbb{R}_T$ ,

$$(2.12) p(T, \cdot) = p^T on \mathbb{R}$$

with terminal data

(2.13) 
$$p^{T}(x) = \begin{cases} \gamma(x)\psi_{y}(y(T,x),y_{d}(x)) & \text{if } y(T,\cdot) \text{ continuous at } x, \\ \gamma(x)\frac{[\psi(y(T,x),y_{d}(x))]}{[y(T,x)]} & \text{if } y(T,\cdot) \text{ discontinuous at } x. \end{cases}$$

Here, [y(T,x)] = y(T,x+) - y(T,x-) and  $[\psi(y(T,x),y_d(x))] = \psi(y(T,x+),y_d(x+)) - \psi(y(T,x-),y_d(x-))$  denote the jumps at x. For the objective functional (1.4) with smoothed observation the terminal data reads

(2.14) 
$$p^T = \phi * (\gamma \psi(\phi * y(T), \phi * y_d)),$$

where we have used the symmetry of the mollifier  $\phi$ . Hence, the smoothed observation ensures Lipschitz end data which leads to a more regular adjoint state and simplifies the convergence analysis of numerical adjoint schemes.

If also rarefaction centers can be controlled, i.e., if (2.9) does not hold, then (2.10) holds with a particular definition of  $p(0, x_j)$  at rarefaction centers obtained by a weighted average over the rarefaction wave, see [81]. For the convergence analysis of discrete adjoint schemes this leads to additional technicalities that will not be reviewed here.

To obtain the representation (2.10), one has to use the unique reversible solution of (2.11)–(2.12). By Oleinik's entropy condition y satisfies under the assumption  $f'' \ge m_{f''} > 0$  a one-sided Lipschitz condition (OSLC) of the form

(2.15) 
$$\partial_x y(t, \cdot) \le \frac{C}{t + 1/\mathrm{Lip}_{\mathbb{R}}^+(u)}, \quad t \in ]0, T],$$

where C > 0 is a constant and the one-sided Lipschitz constant on  $I \subset \mathbb{R}$  open is defined by

$$\operatorname{Lip}_{I}^{+}(u) = \inf\{M \in \mathbb{R} : x \in I \mapsto Mx - u \text{ is monotone increasing}\},$$

see for example [82] for g = 0 and [86] for the general case.

If the initial data u have up-jumps, i.e.  $E := \{z \in \mathbb{R} : [u(z)] > 0\} \neq \emptyset$ , and thus generate a rarefaction wave then  $\operatorname{Lip}_{\mathbb{R}}^+(u) = \infty$  and outside of the set

$$R_{\varepsilon} := \{ (t, x) \in [0, \varepsilon) \times \mathbb{R} : \operatorname{dist}(x, E) \le \varepsilon + M_{f'} t \}, \\ M_{f'} \ge \| f'(y(\cdot, \cdot)) \|_{L^{\infty}(\mathbb{R}_T)} \text{ arbitrary},$$

the OSLC can be refined to

(2.16) 
$$\partial_x y(t,\cdot) \le \frac{2C}{t + \min\{\varepsilon, 1/\operatorname{Lip}^+_{\mathbb{R} \setminus E^{cl}_{\varepsilon}}(u)\}}, \quad (t,x) \in \mathbb{R}_T \setminus R_{\varepsilon}$$

for all  $\varepsilon > 0$ , where  $E_{\epsilon}$  is the  $\varepsilon$ -neighborhood of E. With the convention  $R_{\varepsilon} = \emptyset$  if  $E = \emptyset$ , (2.15) is a special case of (2.16) by setting  $\varepsilon = \infty$ .

Using that  $0 \leq f''(y) \leq ||f''(y)||_{L^{\infty}(\mathbb{R}_T)}$ , we obtain in the case  $E := \{z \in \mathbb{R} : [u(z)] > 0\} = \emptyset$ 

(2.17) 
$$\partial_x f'(y(t,x)) \le \alpha(t), \quad (t,x) \in \mathbb{R}_T, \text{ where } \alpha \in L^1(0,T),$$

and otherwise for all  $\varepsilon > 0$ 

(2.18) 
$$\partial_x f'(y(t,x)) \le \alpha_{\varepsilon}(t), \quad (t,x) \in \mathbb{R}_T \setminus R_{\varepsilon}, \text{ where } \alpha_{\varepsilon} \in L^1(0,T).$$

Again, with the convention  $R_{\varepsilon} = \emptyset$  if  $E = \emptyset$  (2.17) is a special case of (2.18) with  $\alpha_{\varepsilon} = \alpha$ .

As discussed in [28] the solution of (2.11)-(2.12) is not unique if the state contains a shock. To obtain the adjoint representation, a different notion of solution of (2.11)-(2.12) is required that is stable with respect to the coefficient f'(y). It turns out that the reversible solution introduced in [14] with the extension in [86, 87] to discontinuous terminal data yields an appropriate adjoint solution.

In the following, we denote by  $B(\Omega)$ ,  $\Omega \subset \mathbb{R}^n$ , the space of bounded functions equipped with the supremum norm and by  $B(\Omega; Z)$ , Z normed space, the space of bounded functions  $w: \Omega \to Z$  with norm  $||w||_{B(\Omega;Z)} = \sup_{x \in \Omega} ||w(x)||_Z$ . The reason for working with  $B(\Omega; Z)$  instead of  $L^{\infty}(\Omega; Z)$  lies in the fact that the estimates for the adjoint equation hold everywhere and that values of the end data  $p^T$  at shock discontinuities of  $y(T, \cdot)$  determine the reversible solution p of the adjoint equation in the whole shock funnel.

DEFINITION 2.4 (Reversible solution). Let  $p^T \in C^{0,1}_{\text{loc}}(\mathbb{R})$  be arbitrary. Denote by  $\mathcal{L} \subset C^{0,1}_{\text{loc}}(]0,T] \times \mathbb{R}$ ) the set of Lipschitz solutions of (2.11) (i.e., satisfying (2.11) almost everywhere). Then  $p \in \mathcal{L}$  is a reversible solution of (2.11)–(2.12) if p satisfies (2.12) and if there exist  $p_1, p_2 \in \mathcal{L}$  such that  $\partial_x p_1 \ge 0$ ,  $\partial_x p_2 \ge 0$  and  $p = p_1 - p_2$ .

One can show the following existence and uniqueness result [14, 87].

LEMMA 2.5. Let  $p^T \in C^{0,1}_{\text{loc}}(\mathbb{R})$ . Then there exists a unique reversible solution  $p \in C^{0,1}_{\text{loc}}([0,T] \times \mathbb{R})$ . p satisfies

(2.19) 
$$\|p(t,\cdot)\|_{B(I)} \le \|p^T\|_{B(J_t)}$$

for all I = (a, b), a < b, and  $J_t = (a - ||f'(y)||_{L^{\infty}(\mathbb{R}_T)}(T-t), b + ||f'(y)||_{L^{\infty}(\mathbb{R}_T)}(T-t))$ , (including  $a = -\infty$   $b = \infty$ ). Moreover, if the (weakened) OSLC (2.18) holds then

$$\|\partial_x p(t,\cdot)\|_{B(I\setminus\{x:(t,x)\in R_\varepsilon\})} \le e^{\int_t^T \alpha_\varepsilon} \|\partial_x p^T\|_{B(J_t)},$$

where we set  $R_{\varepsilon} = \emptyset$  and  $\alpha_{\varepsilon} = \alpha$  in the case  $E := \{z \in \mathbb{R} : [u(z)] > 0\} \neq \emptyset$ .

The reversible solution can also equivalently be defined along generalized characteristics, see [14].

LEMMA 2.6. Let  $(t,x) \in \mathbb{R}_T$  and denote by  $s \in [t,T] \mapsto X(s;t,x)$  the unique generalized forward characteristic according to Definition 2.2 and (2.8).

Then the reversible solution of Lemma 2.5 can equivalently be obtained from

(2.20) 
$$p(t,x) = p^T(X(T;t,x)), \quad (t,x) \in \mathbb{R}_T.$$

Remark 2.7. Lemma 2.6 provides a convenient interpretation of the reversibel solution. The value  $p^{T}(x)$  is transported along all backward characteristics through (T, x). The OSLC ensures that backward characteristics staring in different points (T, x), (T, y) cannot approach too fast which leads to the Lipschitz continuity of p for Lipschitz continuous end data.

If x is a shock point of  $y(T, \cdot; u)$  then  $p^T(x)$  is propagated along the shock and along all backward characteristics emanating from the shock, which fill the whole shock funnel, i.e. the area between the minimal and the maximal backward characteristic through (T, x). Reversible solutions provide essential stability properties as for example stability with respect to smoothed initial and terminal data. Hence, phas the constant value  $p^T(x)$  in the shock funnel.

Note that any assignment of data along the shock, which are then propagated along backward characteristics emanating from the shock would lead to other solutions of the adjoint equation that are not reversible and not stable with respect to the coefficient.

Since the end data (2.13) can be discontinuous, we need the following extension.

DEFINITION 2.8 (Reversible solution for discontinuous data). If merely

$$p^{T} \in B_{Lip}(\mathbb{R}) := \{ w : \mathbb{R} \to \mathbb{R} : w \text{ is pointwise everywhere the limit of a sequence} \\ (w_{n}) \subset C^{0,1}_{\text{loc}}(\mathbb{R}) \text{ that is bounded in } C(\mathbb{R}) \cap W^{1,1}_{\text{loc}}(\mathbb{R}) \},$$

then a reversible solution of (2.11)–(2.12) is defined by (2.20).

Then the following existence, uniqueness and stability result can be shown [87].

LEMMA 2.9. Let the weakened OSLC (2.18) hold. Then for end data  $p \in B_{Lip}(\mathbb{R})$ there exists a unique reversible solution  $p \in B(\mathbb{R}_T)$  according to Definition 2.8. Moreover, p satisfies the bound (2.19) and

$$p \in B(\mathbb{R}_T) \cap C^{0,1}([0,T]; L^1_{\text{loc}}(\mathbb{R})) \cap B([0,T]; BV_{\text{loc}}(\mathbb{R})) \cap BV_{\text{loc}}([0,T] \times \mathbb{R}).$$

Let p be the reversible solution for terminal data  $p^T$ . Then the following stability property holds. If  $(p_n^T) \subset C_{\text{loc}}^{0,1}(\mathbb{R})$  is bounded in  $C(\mathbb{R}) \cap W_{\text{loc}}^{1,1}(\mathbb{R})$  with  $p_n^T \to p^T$ pointwise and  $p_n \in C_{\text{loc}}^{0,1}(\mathbb{R}_T)$  are the reversible solutions for end data  $p_n^T$ , then  $p_n \to p$ in  $C^{0,1}([0,T]; L_{\text{loc}}^1(\mathbb{R}))$  and for all  $\varepsilon > 0$  one has  $p_n(t,x) \to p(t,x)$  uniformly bounded for all  $(t,x) \in [0,T] \times \mathbb{R} \cup [0,T] \times (\mathbb{R} \setminus E_{\varepsilon})$ .

Remark 2.10. Since reversible solutions transport by (2.20) the terminal data  $p^T$  along backward characteristics, the particular values of the discontinuous data  $p^T$  in (2.13) at the shock locations are propagated within the shock funnel. This poses a challenge for the design and analysis of convergent adjoint discretizations. Moreover, the adjoint state is discontinuous at rarefaction centers.

After the reversible solution of the adjoint equation (2.11)–(2.12) has been defined, we can also characterize measure-valued solutions of the sensitivity equation (2.6) by a duality relation [14, 86]. The following result shows that the differential  $\delta y$  can be expressed in terms of the adjoint variable p. For a definition of  $E_{\epsilon}$  we refer to the line after (2.16).

DEFINITION 2.11 (Duality solution). Let  $S = C([0,T]; \mathcal{M}_{loc}(\mathbb{R}) - weak)$ , where  $\mathcal{M}_{loc}(\mathbb{R}) - weak$  denotes the space  $\mathcal{M}_{loc}(\mathbb{R})$  of locally bounded regular Borel measures on  $\mathbb{R}$  equipped with the weak topology on  $\mathcal{M}_{loc}(\mathbb{R})$  generated by the space  $C_c(\mathbb{R})$ .

Let the weakened OSLC (2.18) hold and let  $\delta u \in \mathcal{M}_{loc}(\mathbb{R}) \cap L^r_{loc}(E_{\varepsilon})$  for some r > 1 and  $\varepsilon > 0$ . Then  $\delta y \in \mathcal{S}$  is called duality solution of (2.6), if for all  $\tau \in ]0,T]$  and all  $p^{\tau} \in C_c^{0,1}(\mathbb{R})$  with the reversible solution of

$$\partial_t p + f'(y)\partial_x p = 0 \text{ on } \Omega_\tau, \quad p(\tau, \cdot) = p^\tau$$

the duality relation holds

$$\int_{\mathbb{R}} p^{\tau} \, \delta y(\tau, \, \mathrm{d}x) = \int_{\mathbb{R}} p(0, x) \, \delta u(\, \mathrm{d}x).$$

By using the properties of the reversible solution, one obtains the following result [14].

LEMMA 2.12. Let the weakened OSLC (2.18) hold. Then for all  $\delta u \in \mathcal{M}_{loc}(\mathbb{R}) \cap L^{r}_{loc}(E_{\varepsilon})$  with some r > 1 and  $\varepsilon > 0$  there exists a unique duality solution  $\delta y \in \mathcal{S}$  of (2.6) and  $\delta y$  satisfies

$$\|\delta y(t,\cdot)\|_{\mathcal{M}(I)} \le \|\delta u\|_{\mathcal{M}(J_t)}$$

for all  $t \in [0, T]$ , I = (a, b), a < b, and  $J_t = (a - ||f'(y)||_{L^{\infty}(\mathbb{R}_T)}t, b + ||f'(y)||_{L^{\infty}(\mathbb{R}_T)}t)$ . Using the duality relation, the adjoint based derivative representation (2.10) of the objective functional can also be expressed by the sensitivity based formula

(2.21) 
$$D_u J(y(u)) \cdot \delta u = \int_{\mathbb{R}} p^T(x) \delta y(T)(\mathrm{d}x) = \int_{\mathbb{R}} p(0, x) \delta u(dx),$$

where  $p^T$  is defined in (2.13) and  $\delta y$  is the duality solution of (2.6) for initial data  $\delta u$ in (2.5). Equation (2.21) is a key equation for numerical approaches of computing a minimizer  $u^*$  since it allows to express the differential of J in terms of adjoint p and control variation  $\delta u$ . An iterative scheme for approximation of  $u^*$  might now utilize the adjoint representation to update the control estimate.

**2.1.1. Further Results.** We give now some pointers to additional results for optimal control theory of scalar conservation laws.

Extensions of the presented results to boundary control problems have been obtained in [76, 81]. Here, analogoulsy as described above for the initial data in addition variations of piecewise  $C^1$  boundary controls are considered, where the boundary condition is understood in the sense of Bardos, LeRoux, Nédélec [7]. Again, a differentiability result similar to Theorem 2.1 can be shown and the derivative of objective functionals of the form (1.3) with respect to initial and boundary controls can be represented by an adjoint formula. To this end, the concept of reversible solutions is extended to initial-boundary value problems leading to boundary conditions for the adjoint equation at the outflow boundaries of the state y.

Optimality conditions for initial-boundary control problems with state constraints and convergence results of penalty methods using Moreau-Yosida regularization have been derived in [81].

By using a non-standard first order variation of BV initial (called shift-differential) data obtained by horizontal shifts of the points of its graph, it is shown in [17] that

the flow generated by a conservation law with strictly convex flux is generically shiftdifferentiable with respect to this differential structure.

There exist also specialized approaches that solve problem (1.1) with g = 0, uniformly convex flux and an objective functional of the form

$$J(y) := \int_{\mathbb{R}} (y(T, x) - y_d(x))^2 \,\mathrm{d}x$$

by a direct backward-forward method without using derivative based optimization methods [70] if  $y_d$  belongs to the attainable set. The advantage lies in the fact that general BV entropy solutions and BV data  $y_d$  can be considered. However, only exact identification can be treated and the approach is only developed for the homogeneous case. In [70] the attainable set and all initial data u leading to an attainable  $y_d$  are characterized. The criterion is closely related to the stationary condition resulting from (2.21) that the adjoint state should vanish at t = 0, i.e.  $p(0, \cdot) = 0$ . Moreover, a backward-forward method for the computation of the optimal solution u leading to the attainable end data  $y_d$  is developed.

A similar approach (1.1) with g = 0 and uniformly convex flux based on the Hopf-Lax-Oleinik explicit formula is proposed in [1]. Here, it is not required that  $y_d$  is attainable but the particular objective functional  $J(y) := \int_{\mathbb{R}} (f'(y(T, x)) - f'(y_d(x)))^2 dx$ is considered. In this case it is shown that (1.1) is equivalent to a convex optimization problem and a backward construction algorithm of its solution is proposed. Again, no additional regularity assumptions are required, but the approach is limited to a very particular instance of (1.1).

To obtain efficient descent methods for the optimal control of conservation laws, [22, 66] propose an alternating descent method for the optimal control of Burgers' equation and the shallow-water equations [72]. It alternates the descent directions corresponding to the shock sensitivities to move the shock and those of the smooth parts between the shocks to produce fast descent algorithms. In [23] the method is considered for the viscous case and it is shown that the optimal controls converge to those of the inviscid case as the viscosity parameter tends to zero. An extension to general scalar conservation laws with uniformly convex flux function should be possible. In the case of hyperbolic systems it is known that the limit depends on the particular form of the viscosity added to the system. A corresponding result is therefore not expected.

The convergence of sensitivities and adjoints for viscous approximations of conservation laws in the vanishing viscosity limit has been shown in [75].

Results on the optimal control of conservation laws with monotone but discontinuous local fluxes can be found in [65, 34]. The case of optimal control for local flux functions has been discussed e.g. in [24], and for nonlocal flux functions e.g. in [34, 32].

Steady-state problems have been analysed e.g. in [41].

2.2. System's Case. A calculus for first-order variations of piecewise Lipschitz continuous solutions of hyperbolic systems (1.2) that contain finitely many discontinuities has been proposed in [19]. We will recall the necessary definitions and state the main result in Theorem 2.16 below. Corresponding optimality conditions have been derived in [20, 18]. Here, the variations of the initial data are of the same type (2.2) as discussed for the scalar case, but only directional variations are considered. This approach will be introduced below. An alternative variational calculus based on horizontal shifts of initial controls in BV, which we will not discuss in detail, has been

extended from the scalar case [17] to the systems case in [12].

As an analytical foundation for sensitivity calculations in the case of hyperbolic systems, we sketch now a fundamental result of [19, Theorem 2.2]. Following [19] we consider piecewise Lipschitz functions of the form (2.1) and allow for variations of the discontinuities and the smooth parts.

DEFINITION 2.13 (Generalized tangent vector). Consider a piecewise Lipschitz continuous function  $u : [a,b] \to \mathbb{R}^n$  of the form (2.1) with jumps at the points  $a < x_1 < \ldots < x_N < b$  and denote by  $\Sigma_u$  the family of all continuous paths  $\gamma : [0, \delta_0] \mapsto L^1([a,b];\mathbb{R}^n)$  with  $\gamma(0) = u$ .

The space of generalized tangent vectors to u is defined as  $T_u := L^1([a, b]; \mathbb{R}^n) \times \mathbb{R}^N$ . A continuous path  $\gamma \in \Sigma_u$  generates the tangent vector  $(v, \xi) \in T_u$  if the path

$$\gamma_{(v,\xi;u)}(\delta) := u + \delta \cdot v + \sum_{\xi_{\alpha} < 0} [u(x_{\alpha})] \mathbf{1}_{[x_{\alpha} + \xi_{\alpha}\delta, x_{\alpha}]} - \sum_{\xi_{\alpha} > 0} [u(x_{\alpha})] \mathbf{1}_{[x_{\alpha}, x_{\alpha} + \xi_{\alpha}\delta]}$$

is equivalent to  $\gamma$  in the sense that

$$\lim_{\delta \to 0+} \frac{1}{\delta} \| \gamma(\delta) - \gamma_{(v,\xi;u)}(\delta) \|_{L^1} = 0.$$

The choice of  $T_u$  reflects possible variations in the values of u as well as possible shifts in the positions  $x_i$  of the N jump discontinuities, see also equation (2.1).

For the variation of initial data, continuous paths  $\gamma$  with  $\gamma(0) = u$  are considered that preserve the piecewise Lipschitz structure.

DEFINITION 2.14 (Regular variation). A piecewise Lipschitz continuous function  $u : [a,b] \to \mathbb{R}^n$  of the form (2.1) with jumps at the points  $a < x_1 < \ldots < x_N < b$  is in the class PLSD of Piecewise Lipschitz functions with simple discontinuities, if each jump of u consists of a contact discontinuity or of a single, stable shock (see [19, Definition 2]).

Let u be a PLSD function. A path  $\gamma \in \Sigma_u$  is a Regular Variation for u, if all functions  $u_{\delta} := \gamma(\delta), \ \delta \in [0, \delta_0]$ , are in PLSD with jumps at points  $a < x_1^{\delta} < \ldots < x_N^{\delta} < b$  depending continuously on  $\delta$  and having a Lipschitz constant between the jumps independently of  $\delta$ .

Hence, if  $\gamma$  is a regular variation of a PLSD function u and  $(v, \xi) \in T_u$  is a generalized tangent vector then  $\xi_{\alpha}$  provide derivatives for the shock locations  $x_{\alpha}^{\delta}$  at  $\delta = 0$  and v a derivative in  $L^1$  for the Lipschitz parts  $u_{\delta}|_{[x_{\alpha-1}+\varepsilon,x_{\alpha}-\varepsilon]}$  at  $\delta = 0$  for all  $\varepsilon > 0$  small enough. For more details we refer to [19].

It is now shown in [19, Theorem 2.2] that regular variations of the initial data u are locally preserved by the system of conservation laws (1.2) and that generalized tangent vectors can be obtained by an appropriate linearized equation. To state this result, we recall the definition of broad solutions of semi-linear systems.

DEFINITION 2.15 (Broad solution). Consider the semi-linear partial differential equation

(2.22) 
$$y_t(t,x) + A(t,x)y_x(t,x) = g(t,x,y),$$

where  $A \in \mathbb{R}^{n \times n}$  is strictly hyperbolic, Lipschitz and g is measurable with respect to (t, x) and Lipschitz continuous with respect to y. Assume an initial condition y(0, x) = u(x) with  $u \in L^1(\mathbb{R}; \mathbb{R}^n)$ . Denote by  $\ell_i, r_i$  the ith left and right eigenvectors of A.

Denote by  $\lambda_i$  the *i*th eigenvalues of A. We denote by  $t \to z_i(t; \tau, \xi)$  the solution to the Cauchy problem

(2.23) 
$$\frac{d}{dt}z(t) = \lambda_i(t, z(t)), \ z(\tau) = \xi.$$

Denote by  $\langle \cdot, \cdot \rangle$  the scalar product on  $\mathbb{R}^n$  and by

$$g_i := \langle \ell_i, g \rangle + \langle \partial_t \ell_i + \lambda_i \partial_x \ell_i, y \rangle, \ y = \sum_{i=1}^n y_i r_i.$$

We define a broad solution  $y = \sum_{i=1}^{n} y_i r_i$  to equation (2.22) as a locally integrable function fulfilling

$$\frac{d}{dt}y_i(t, z_i(t; \tau, \xi)) = g_i(t, z_i(t; \tau, \xi), y(t, z_i(t; \tau, \xi)))$$

in the sense that for a.e. $(\tau, \xi)$  and all  $i = 1, \ldots, n$  the following holds

$$y_i(\tau,\xi) = u_i(z_i(0;\tau,\xi)) + \int_0^\tau g_i(s, z_i(s;\tau,\xi), y(s, z_i(s;\tau,\xi))) \, ds.$$

Note that equation (2.23) are the characteristics and the values are propagated with the local eigenvalues  $\lambda_i$ . If strict hyperbolicity of A is imposed, the eigenvalues  $\lambda_i$  are simple and depend as A Lipschitz continuously on (t, x). Hence, the characteristics  $z_i$  are well defined and  $C^1$ . This leads to assumptions (H1) and (H2). Further, assumption (H3) guarantees that the linearized Rankine Hugoniot jump conditions can be solved uniquely with respect to the outgoing variables.

(H1) The vector field  $f: \Omega \to \mathbb{R}^n$  is  $\mathcal{C}^2$ 

where  $\Omega \subset \mathbb{R}^n$  is closed and bounded. For each  $y \in \Omega$  the matrix A(y) = Df(y) has *n* real distinct eigenvalues. Its eigenvalues  $\lambda_i$  are increasingly ordered and its left and right eigenvectors  $\ell_i$  and  $r_i$ , respectively, are normalized such that  $\langle \ell_i, r_j \rangle = \delta_{ij}$ . Let

$$A(u,v) = \int_0^1 A(\theta u + (1-\theta)v)d\theta$$

with corresponding eigenvectors  $\ell_i(u, v)$ ,  $r_i(u, v)$  and eigenvalues  $\lambda_i(u, v)$ . Suppose that  $\ell_i(u, v)$ ,  $r_i(u, v)$  and  $\lambda_i(u, v)$  are uniformly bounded for all  $u, v \in \Omega$ .

(H2) Denote by  $\hat{\lambda}$  the uniform bound on  $\lambda_i(i, v)$  for all *i*. Then, solutions to (2.22) are considered in the domain

$$\mathcal{D} := \{(t, x) : 0 \le t \le T, x \in [a + \hat{\lambda}t, b - \hat{\lambda}t]\}$$

Assume further that the function  $g: \mathcal{D} \times \Omega \to \mathbb{R}^n$  is bounded and continuously differentiable.

(H3) Whenever  $y^+ \in \Omega$  and  $y^- \in \Omega$  are connected by a shock or a contact discontinuity, say of the kth characteristic family, the linear system

$$0 = \Phi_i(y^+, y^-, v^+, v^-) = \sum_{j=1}^n \langle D\ell_i(y^+, y^-) \cdot (v_j^+ r_j^+, v_j^- r_j^-), y^+ - y^- \rangle + \sum_{j=1}^n \langle \ell_i(y^+, y^-), v_j^+ r_j^+ - v_j^- r_j^- \rangle, \ \forall i \neq k$$

can be uniquely solved in terms of the outgoing variables  $v_{j^{\pm}}^{\pm} j^{\pm} \in \{j^{-} : j < k\} \cup \{j^{+} : j > k\} =: \mathcal{O}$ . Further assume, that the function  $W_{j}$  defined by

$$v_j^{\pm} = W_{j^{\pm}}(y^+, y^-)((v_j)_{j^{\pm} \notin \mathcal{O}}), \ j \neq k, j^{\pm} \in \mathcal{O}$$

satisfies a bound of the form

$$||W_{j^{\pm}}(y^{+}, y^{-})((v_{j})_{j^{\pm} \notin \mathcal{O}})|| \leq C ||(v_{j})_{j^{\pm} \notin \mathcal{O}}||.$$

Here,  $r_j^{\pm} = r_j(u^{\pm})$ . Then the following result is shown in [19, Theorem 2.2]. Note that the solution y and  $y_{\delta}$  are in the class PLSD. Hence, between discontinuities the functions are Lipschitz and equation (2.24) is only defined therein. The solution y is assumed to have  $\alpha = 1, \ldots, N$  discontinuities located at  $x_{\alpha}$ .

THEOREM 2.16. Let the assumptions (H1)–(H3) hold true. Let y be a piecewise Lipschitz continuous solution to equation (1.2) with  $u(0, \cdot) = u$  in the class PLSD. Let  $(v_0, \xi_0) \in L^1 \times \mathbb{R}^N$  be a tangent vector to u generated by a regular variation  $\gamma_0 : \delta \mapsto u_{\delta}$ , Let  $y_{\delta}$  be the solution of equation (1.2) with initial condition  $u_{\delta}$ . Then, there exists  $\tau_0 > 0$  such that for all  $t \in [0, \tau_0]$  the path  $\gamma_t : \delta \mapsto y_{\delta}(t, \cdot)$  is a regular variation for  $y(t, \cdot)$  generating the tangent vector  $(v(t), \xi(t)) \in L^1 \times \mathbb{R}^N$ . The vector is the unique broad solution of the initial boundary value problem

(2.24) 
$$\xi(0) = \xi_0, v(0, x) = v_0(x),$$

(2.25) 
$$v_t + A(y)v_x + (DA(y)v)y_x = g_y(t, x, y)v,$$

outside the discontinuities of y while for  $\alpha = 1, \ldots, N$ 

(2.26) 
$$\langle D\ell_i(y^+, y^-) \cdot (v^+ + \xi_{\alpha} y_x^+, v^- + \xi_{\alpha} y_x^-), y^+ - y^- \rangle + \langle \ell_i(y^+, y^-), v^+ + \xi_{\alpha} y_x^+ - v^- - \xi_{\alpha} y_x^- \rangle = 0, \quad \forall i \neq k_{\alpha},$$
(2.27) 
$$\frac{d}{dt} \xi_{\alpha} = D\lambda_{k_{\alpha}}(y^+, y^-)(v^+ + \xi_{\alpha} y_x^+, v^- + \xi_{\alpha} y_x^-)$$

along each line  $x = x_{\alpha}(t)$  where y suffers a discontinuity in the  $k_{\alpha}$  characteristic direction. Here,  $y^+, v^+$  and  $y^-, v^-$  denote the right and left traces of y, v along  $x = x_{\alpha}(t)$ , respectively.

Note that (2.26) and (2.27) result form the linearization of the Rankine-Hugoniot jump condition. The evolution of tangent vetors can be continued beyond times, where shocks interact. For details we refer to [19].

Finally, note that there exist also formal derivations of sensitivities and adjoints for piecewise smooth solutions of systems with a single shock also for several space dimensions, see e.g. [9] and also [67]. Under the assumption that the shock and the solution to both sides of the shock depend differentiable on a parameter, a parametrization of the shock curve is added as state variable and sensitivity equations away form the shock and along the shock are derived. Moreover, an adjoint equation away form the shock with an interior boundary condition along the shock is obtained. The results are applied to the p-system.

To the best of our knowledge approaches using viscosity on systems of conservation laws and their corresponding differential calculus in the zero viscosity limit have not been discussed. **3. Numerical Analysis.** We introduce a spatial grid on  $\mathbb{R}$  with cell centers  $x_i$  for  $i \in \mathbb{Z}$  and cells  $C_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$  where for simplicity  $\Delta x = x_{i+1} - x_i > 0$  is fixed for all *i*. In the fully discrete case a temporal grid  $t_n = n\Delta t$  with  $n \in \mathbb{N}$  is introduced and the cell average of a function  $y(t, \cdot) \in L^1(\mathbb{R})$  at time *t* and  $t = t^n$  is denoted by

(3.1) 
$$y_i(t) = \frac{1}{\Delta x} \int_{C_i} y(t, x) \, \mathrm{d}x \text{ and } y_i^n = \frac{1}{\Delta x} \int_{C_i} y(t^n, x) \, \mathrm{d}x, i \in \mathbb{Z},$$

respectively. The time step  $\Delta t$  is  $\Delta t = \lambda \Delta x$ , where  $\lambda > 0$  is chosen such the CFL condition holds. If not stated otherwise, a numerical solution is obtained as piecewise constant approximation  $y_h(t, x)$  of y given by

(3.2) 
$$y_h(t,x) = \sum_{n \ge 0} \sum_{i \in \mathbb{Z}} \chi_{[t^n, t^{n+1}] \times C_i}(t,x) y_i^n.$$

The subscript h denotes the numerical approximation of the corresponding quantity. Hence, given any function  $v \in L^1_{loc}(\mathbb{R})$ , we obtain a grid function  $A_h v$  by the averaging operator

$$(A_h v)(x) = \frac{1}{\Delta x} \int_{C_i} v(\xi) \, d\xi \quad \text{for } x \in C_i.$$

**3.1. First-Order Finite-Volume Schemes.** Let  $N_T$  be defined such that  $T \in [t_{N_T}, t_{N_T+1})$  (analogously, we define  $N_t$  for  $t \in (0, T]$ ). To discretize the state equation (1.2) we start by considering first-order finite-volume schemes (which can also be interpreted as conservative finite difference schemes) of the form

(3.3) 
$$y_i^{n+1} = y_i^n - \lambda \Delta^- F_{i+\frac{1}{2}}^n := H(y_{i-K}^n, \dots, y_{i+K}^n), \quad i \in \mathbb{Z}, \ n = 0, \dots, N_T - 1,$$
$$y_i^0 = u_i, \quad i \in \mathbb{Z},$$

for a stencil of width  $K \ge 1$ , where

$$F_{i+\frac{1}{2}}^{n} = F(y_{i-K+1}^{n}, \dots, y_{i+K}^{n}), \quad \Delta^{-}F_{i+\frac{1}{2}}^{n} = F_{i+\frac{1}{2}}^{n} - F_{i-\frac{1}{2}}^{n}$$

with a consistent numerical flux F, i.e.,

(3.4) 
$$F \in C^{1,1}_{\text{loc}}(\mathbb{R}^{2K};\mathbb{R}^n), \quad F(y,\ldots,y) = f(y) \text{ for all } y \in \mathbb{R}^n.$$

For concreteness, the control  $u \in L^{\infty}(\mathbb{R})$  is approximated by the cell averages

(3.5) 
$$u_h(x) = (A_h u)(x), \quad u_i = (A_h u)(x_i).$$

The grid function  $y_h$  corresponding to  $y_i^n$  approximates the entropy solution y. The discrete control-to-state mapping is thus

$$(3.6) u_h \longmapsto y_h.$$

As discrete approximation of the objective functional J in (1.3) we choose for example

(3.7) 
$$u_h \longmapsto J^h(y_h) := \int_{\mathbb{R}} \gamma_h(x) \psi(y_h(T, x), y_{d,h}(x)) \, \mathrm{d}x = \sum_i \Delta x \, \gamma_i \, \psi(y_i^{N_T}, y_{d,i}),$$

where  $\gamma_h = A_h \gamma$  and  $y_{d,h} = A_h y_d$  with associated grid values  $\gamma_i, y_{d,i}$ . In the case of the objective functional (1.4) with smoothed observation we consider for simplicity

(3.8)  
$$u_{h} \longmapsto J^{s,h}(y_{h}) := \int_{\mathbb{R}} \gamma_{h}(x)\psi((\phi \ast_{h} y_{h}(T))(x), (\phi \ast_{h} y_{d,h})(x)) dx$$
$$= \sum_{i} \Delta x \gamma_{i} \psi((\phi \ast y_{h}(T))(x_{i}), (\phi \ast y_{d,h})(x_{i})),$$

where  $(\phi *_h y_h(T))(x) = (\phi * y_h(T))(x_i)$  for  $x \in C_i$ .

By the above assumptions the discrete control-to-state mapping (3.6) and consequently also the discrete objective functional (3.7) is continuously differentiable. The derivative is obviously given by

$$(3.9) D_{u_h} y_h(u_h) \cdot \delta u_h = \delta y_h,$$

where  $\delta y_h$  is the discrete sensitivity and its grid values  $\delta y_i^n$  solve the discrete sensitivity equation obtained by linearizing the scheme (3.3)

(3.10) 
$$\delta y_i^{n+1} = \delta y_i^n - \lambda \sum_{k=1-K}^K \Delta^- (F_{y_k,i+\frac{1}{2}}^n \delta y_{i+k}^n),$$
$$\delta y_i^0 = \delta u_i,$$

where  $\lambda = \frac{\Delta t}{\Delta x}$  is chosen such that the CFL condition holds and

$$F_{y_k,i+\frac{1}{2}}^n = F_{y_k}(y_{i+1-K},\dots,y_{i+K})$$

and  $F_{y_k}$ ,  $k = 1 - K, \ldots, K$ , denotes the partial derivative of  $F(y_{1-K}, \ldots, y_K)$  with respect to the (k + K)-th argument  $y_k$ . Using (3.9), it is obvious that

(3.11) 
$$D_{u_h} J^h(y_h(u_h)) \cdot \delta u_h = \int_{\mathbb{R}} \gamma_h(x) \partial_y \psi_y(y_h(T, x), y_{d,h}(x)) \, \delta y_h(T, x) \, \mathrm{d}x$$
$$= \sum_i \Delta x \gamma_i \partial_y \psi(y_i^{N_T}, y_{d,i}) \, \delta y_i^{N_T},$$

(3.12)

$$D_{u_h}J^{s,h}(y_h(u_h)) \cdot \delta u_h = \int_{\mathbb{R}} (\phi *_h (\gamma_h \partial_y \psi(\phi *_h y_h(T), (\phi *_h y_{d,h})))(x) \delta y_h(T, x) \, \mathrm{d}x$$

with the sensitivities  $\delta y_h$  and corresponding grid values  $\delta y_i^n$  according to (3.10). Here, the symmetry of the mollifier  $\phi$  has been used in the last equation.

By applying standard adjoint calculus one obtains the adjoint representation of the derivative [79]

(3.13) 
$$D_{u_h} J^h(y_h(u_h)) \cdot \delta u_h = \Delta x \sum_i p_i^0 \, \delta u_i,$$

where  $p_i$  are the point values of  $p_h$  that solves the discrete adjoint equation

(3.14) 
$$p_i^n = p_i^{n+1} + \lambda \sum_{k=1-K}^K (F_{i-k+\frac{1}{2},k}^n) \Delta^+ p_{i-k}^{n+1}, \quad i \in \mathbb{Z}, \ n = 0, \dots, N_T - 1,$$

(3.15) 
$$p_i^{N_T} = \gamma_i \nabla_y \psi(y_i^{N_T}, y_{d,i}), \quad i \in \mathbb{Z},$$

where  $\Delta^{+} p_{i}^{n+1} = p_{i+1}^{n+1} - p_{i}^{n+1}$ .

A derivative representation of the form (3.13) holds also for (3.8), where the end data (3.15) are replaced by

(3.16) 
$$p_h(T) = \phi *_h (\gamma_h \nabla_y \psi(\phi *_h y_h(T), y_{d,h})).$$

**3.2. Scalar Case.** For the scalar case with uniformly convex flux function, i.e.  $f'' \ge m_{f''} > 0$ , the convergence properties of discrete adjoints is nowadays quite well understood. To state suitable CFL conditions, it will be useful to define the coefficients for  $i \in \mathbb{Z}$  and  $n \in \mathbb{N}$  and  $K \ge 1$  being the width of the stencil:

$$(3.17) \qquad \begin{aligned} a_{i+\frac{1}{2},k}^{n} &= F_{y_{k},i+\frac{1}{2}}, \\ B_{i,k}^{n} &= \delta_{0,k} + \lambda (a_{i-k-\frac{1}{2},k+1}^{n} - a_{i-k+\frac{1}{2},k}^{n}), \quad -K < k < K, \\ B_{i,-K}^{n} &= \lambda a_{i+K-\frac{1}{2},1-K}^{n}, \quad B_{i,K}^{n} &= -\lambda a_{i-K+\frac{1}{2},K}^{n}, \\ C_{i,k}^{n} &= B_{i,k}^{n} + \lambda \Delta^{-} a_{i-k+\frac{1}{2},k+1}^{n}, \quad -K \leq k < K, \\ C_{i,K}^{n} &= B_{i,k}^{n} + \lambda \Delta^{-} a_{i-k+\frac{1}{2},k+1}^{n}, \quad -K \leq k < K, \\ \end{aligned}$$

Then for scalar problems the adjoint scheme (3.14) can be written in the following forms

(3.18) 
$$p_i^n = \sum_{k=-K}^K B_{i,k}^n p_{i-k}^{n+1}, \quad \Delta^+ p_i^n = \sum_{k=-K}^K C_{i,k}^n \Delta^+ p_{i-k}^{n+1}.$$

The convergence analysis of discrete adjoint schemes (3.14) poses two main challenges. Firstly, convergence to the reversible solution has to be shown.

Secondly, as noted in Remark 2.10 the values of the discontinuous end data  $p^T$  in (2.13) at the shock locations are propagated within the shock funnel while in (3.14) some averaging over the discrete shock profile takes place and it is quite involved to study this averaging process. Schemes of the form (3.18) for homogeneous transport equations have been analyzed in [47], but not in the context of optimal control such that the coefficients do not depend on a discrete state. The extension to adjoint equations in optimal control has been studied in [85, 79, 80].

Rigorous results have so far mainly been obtained for adjoint schemes corresponding to monotone schemes (3.3), i.e.,

(3.19) 
$$H(y_{i-K}^n, \dots, y_{i+K}^n)$$
 is nondecreasing in each argument.

This comprises the Engquist-Osher scheme with numerical flux

$$F^{\rm EO}(y_0, y_1) = f(\bar{y}) + \int_{\bar{y}}^{y_0} \max(f'(y), 0) \, dy + \int_{\bar{y}}^{y_1} \min(f'(y), 0) \, dy,$$

where  $\bar{y} \in \mathbb{R}$  is fixed and the modified Lax-Friedrichs or Rusanov scheme with numerical flux

(3.20) 
$$F^{\mathrm{LF}}(y_0, y_1) = \frac{1}{2} \left( f(y_0) + f(y_1) - \frac{\nu}{\lambda} (y_1 - y_0) \right), \quad \nu \in [\lambda \max_{y \in [y_0, y_1]} |f'(y)|, 1),$$

where the maximum is taken over the whole region in which  $y_0, y_1$  vary. The classical Lax-Friedrichs scheme corresponds to  $\nu = 1$ , but for the convergence of the adjoint scheme  $\nu < 1$  is required. Then under a suitable CFL condition it can be ensured that the coefficients in (3.17) satisfy  $B_{i,k}^n \geq 0$  and  $C_{i,k}^n \geq 0$ . The classical Lax-Friedrichs

decouples the computation of  $y_i^n$  for even and odd i and does not ensure that the coefficient  $C_{i,0}^n$  is nonnegative, which prohibits a BV-estimate for the discrete adjoint.

Moreover, it is well known that many monotone schemes such as the modified Lax-Friedrichs scheme and the Engquist-Osher scheme [69] the discrete state  $y_h$  satisfies under a suitable CFL condition in analogy to (2.16) a discrete one-sided Lipschitz condition of the form, see e.g. [74, 82],

(3.21) 
$$\frac{\Delta^+ y_i^n}{\Delta x} \le \frac{2C}{t + \min\{\varepsilon, 1/\operatorname{Lip}^+_{\mathbb{R} \setminus E_\varepsilon^{cl}}(u)\}}, \quad (t_n, x_i), (t_n, x_{i+1}) \in \mathbb{R}_T \setminus R_\varepsilon$$

with  $M_{f''} = 1/\lambda$  in the definition of  $R_{\varepsilon}$  and the convention that  $R_{\varepsilon} = \emptyset$  and  $\varepsilon = \infty$ if  $E := \{z \in \mathbb{R} : [u(z)] > 0\} = \emptyset$ .

This motivates the following assumption, that allows us to cover 1) the discretizethen-optimize approach where (3.14) is chosen as discrete adjoint scheme of the discrete state equation (3.3), 2) the optimize-the-discretize approach, where an adjoint scheme of the form (3.14) is used, but the state is computed by another convergent scheme. We make the following assumption on the state and the flux function used in (3.14).

- (H4) 1.  $F \in C^{1,1}_{\text{loc}}(\mathbb{R}^{2K})$  and is consistent with f, i.e., (3.4) holds. 2. With constants  $h_0, M_y > 0$  and the entropy solution y = y(u) of (1.2)
  - for all  $h = \Delta x = \Delta t / \lambda \leq h_0$  it holds for all  $t \in [0, T]$

$$||y_h||_{L^{\infty}(\mathbb{R}_T)} \leq M_y, \ y_h(t,\cdot) \to y(t,\cdot) \text{ in } L^1_{loc}(\mathbb{R}) \text{ as } h \to 0,$$
  
 $\partial_{y_k} F \text{ are on } [-M_y, M_y]^{2K} \text{ nondecreasing in each argument.}$ 

3. With a function  $\beta_{\varepsilon} \in L^1(0,T)$  and some  $h_0 > 0$  for all  $h = \Delta t/\lambda \leq h_0$ the discrete one-sided Lipschitz condition holds

$$(3.22) \qquad \frac{\Delta^+ y_i^n}{\Delta x} \le \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} \beta_{\varepsilon}(t) \, \mathrm{d}t \quad \forall (t_n, x_i), (t_n, x_{i+1}) \in \mathbb{R}_T \setminus R_{\varepsilon}$$

with some  $M_{f''}$  in the definition of  $R_{\varepsilon}$  and the convention that  $R_{\varepsilon} = \emptyset$ and  $\varepsilon = \infty$  if  $E := \{z \in \mathbb{R} : [u(z)] > 0\} = \emptyset$ .

We note that (H4) is satisfied for the Engquist-Osher scheme under a 1/2-CFL condition and for the modified Lax-Friedrichs scheme under a min( $\nu$ , 1 –  $\nu$ )-CFL condition [35, 74, 79]. In particular, (3.22) is implied by (3.21).

We collect now some convergence results for different scenarios. The first result addresses the objective functional with smoothed observation (1.4) and its discretization (3.8) and follows from results in [79].

THEOREM 3.1. Let (H4) hold. Consider the discrete objective function (3.8) with discrete gradient representation (3.13) based on the adjoint scheme (3.14), (3.16) (if  $y_h$  is generated by the state scheme (3.3) corresponding to (3.14) the representation is exact).

Let a CFL condition hold such that the coefficients  $B_{ik}^n, C_{ik}^n$  in (3.17) satisfy

 $B_{i,k}^n, C_{i,k}^n \ge 0, \quad -K \le k \le K, \quad for \ all \ i \in \mathbb{Z}, \quad 0 \le n \le N_T - 1.$ 

Then the solution of the adjoint scheme (3.14), (3.16) satisfies

$$\|p_h\|_{L^{\infty}(\mathbb{R}_T)} \le \|p_h(T)\|_{L^{\infty}(\mathbb{R})}$$
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and the discrete Lipschitz estimate

$$\frac{|\Delta^+ p_i^n|}{\Delta x} \le \sup_i \frac{|\Delta^+ p_i^{N_T}|}{\Delta x} e^{\int_{t_n}^{t_{N_T}} \beta_{\varepsilon}(s) \, ds} \forall \, (t_n, x_i), (t_n, x_{i+1}) \in \mathbb{R}_T \setminus R_{\varepsilon}$$

with  $R_{\varepsilon}$  as in (H4) and the convention that  $R_{\varepsilon} = \emptyset$  and  $\varepsilon = \infty$  if  $E := \{z \in \mathbb{R} : |u(z)| > 0\} = \emptyset$ .

Moreover,  $p_h$  converges on  $\mathbb{R}_T \setminus R_{\varepsilon}$  for all  $\varepsilon > 0$  locally uniformly to the unique reversible solution  $p \in B(\mathbb{R}_T) \cap C^{0,1}(\mathbb{R}_T \setminus R_{\varepsilon})$  of the adjoint equation (2.11) with end data (2.14).

In particular, the discrete gradient approximation  $p_h(0)$  of  $J^{s,h}$  in (3.8), (3.13) converges locally uniformly on  $\mathbb{R} \setminus E_{\varepsilon}$  to the gradient representation p(0) of  $J^s$  in (1.4), (2.10).

As already mentioned, the previous Theorem applies in particular to the Engquist-Osher scheme under a 1/2-CFL condition and for the modified Lax-Friedrichs scheme under a min $(\nu, 1 - \nu)$ -CFL condition.

Next we turn to objective functionals J(y) in (1.3) without smoothing. Then the additional challenge arises that the values of the discontinuous end data  $p^T$  in (2.13) at the shock locations have to be propagated in the shock funnel which requires an appropriate averaging across the discrete shock profile. One possible solution are schemes with numerical viscosity of order  $O(h^{\rho})$ ,  $2/3 < \rho < 1$ , at shocks. We follow [44, 45] and make the following assumption.

(H5)  $f \in C^{\infty}(\mathbb{R}), f'' \geq m_{f''} > 0, g \equiv 0, ||u||_{L^{\infty}(\mathbb{R})} < \infty$ . Moreover, denoting by  $X_0$  the set of points x for which the characteristics propagate up to the final time T without entering a shock, i.e.,  $X_0 = \{x : y(x + f'(u(x))t, t) = u(x), 0 < t < T\}$ , there exists an open set  $X_1$  containing  $X_0^{cl}$  such that u(x)is  $C^{\infty}$  on  $X_1$ , all of its derivatives have a finite  $L^1$  norm on  $X_1$ , and

$$f''(u(x))u'(x) > -\frac{1}{T} \quad \forall x \in X_1^{cl}.$$

The second part of the assumption ensures that no new shocks form at time T, preexisting shocks have a smooth behavior in an open neighborhood of T, and between the shocks the solution y(T, x) is smooth.

Then for a modified Lax-Friedrichs scheme with numerical viscosity of order  $O(h^{\rho})$ ,  $2/3 < \rho < 1$ , the following was shown in [44, 45] by a careful asymptotic expansion with respect to the numerical viscosity.

THEOREM 3.2. Consider the optimal control problem (1.1) with objective functional (1.3) and its discretization by a modified Lax-Friedrichs scheme (3.3), (3.20) with

$$0 < \nu < 1, \quad \Delta t = \frac{T}{N_T} = \frac{\nu}{2} \Delta x^{2-\rho}, \quad 2/3 < \rho < 1,$$

and discrete objective functional (3.7). Let (H5) hold true. Then for  $h \rightarrow 0$  the following holds.

Outside of the extreme backward characteristics emanating form shocks at time Tthe error in the discrete adjoint is  $|p(0,x)-p_h(0,x)| = O(h^{\rho})$  for all  $x \in \mathbb{R}$ . Moreover, within the shock region (more precisely, within any subdomain with positive distance from its two bounding characteristics) the discrete adjoint is constant to within  $o(h^q)$ , for any q > 0, and the error to the correct constant value of the adjoint is  $O(h^{\rho})$ . Remark 3.3. It should be possible to extend the result to schemes that use a numerical viscosity of  $O(h^{\rho})$ ,  $2/3 < \rho < 1$ , only in a sufficiently large vicinity of the shocks.

In [45] an example is presented that shows that with a numerical viscosity of O(h) convergence of the discrete adjoint  $p_h$  to the correct value within the shock funnel is in general not ensured. This is for example the case for the classical Lax–Friedrichs scheme. Hence, a modified diffusion needs to be taken into account as shown in the previous Theorem. Therefore, a naive discretization leads usually to the wrong derivative concerning the contribution of the sensitivity of the shock locations to the derivative of the objective functional. As the example in [45] illustrates, the obtained discrete adjoint need not even provide a descent direction within the shock funnels.

To obtain convergent discrete adjoints for objective functionals J(y) in (1.3) without using a scheme with numerical viscosity  $O(h^{\rho})$ ,  $2/3 < \rho < 1$ , it is also possible to modify the end data of the adjoint scheme in a vicinity of shocks appropriately. A possible procedure that ensures convergence of the discrete adjoint within the shock funnels to the correct value, is described as follows.

We make the following assumption that is in particular satisfied for monotone schemes, see [64].

(H5) Assume that for  $u \in BV(\mathbb{R})$  there exists a constant C(t) > 0 such that

$$\|y^{h}(t, \cdot; u_{h}) - y(t, \cdot; u)\|_{L^{1}(\mathbb{R})} \leq C(t) \|u\|_{TV} h^{1/2} \quad \forall t \in [0, T], \ 0 < h \leq h_{0}.$$

Using an interpolation inequality between the one-sided Lipschitz norm and the  $L^1$ norm, one can show the following, see [74]. Here,  $h_0$  is as in assumptions (H4), (H5).

THEOREM 3.4. Let  $u \in BV(\mathbb{R})$  (H5) hold and let  $y_h$  satisfy the discrete OSLC (3.22). Then for any t > 0 and  $x \in \mathbb{R}$  there exists a constant C(t) > 0 such that

$$|y(t,x) - y_h(t,x)| \le C(t) \left(1 + \max_{|\xi - x| \le h^{1/3}} |\partial_x y(t,\xi)|\right) h^{1/3}$$

 $O(h^{1/3})$  is the best known pointwise convergence rate that can be obtained to hold up to a distance of the same order from discontinuity points of y. It follows by a careful usage of the one-sided Lipschitz continuity and a balancing of the  $L^1$ convergence rate  $O(h^{1/2})$  with the considered distance to discontinuity points of y.

Assume that  $y(T, \cdot)$  has shock locations at  $x_1, \ldots, x_K$  and that  $y_h$  satisfies (H4), (H5). To estimate  $x_1, \ldots, x_K$  from the discrete solution  $y_h$  we determine the K regions, where  $\Delta^+ y_j^{N_{\bar{t}}} = -O(\sqrt{h})$  and choose  $x_k^h$  as the middle point  $x_{i_k}$  of the k-th region. We approximate  $p^T(x_k)$  in (2.13) by

$$p_{x_k^h}^T = \gamma(x_k^h) \frac{\psi(y_h(T, x_k^h + h^{1/3}), y_d(x_k^h)) - \psi(y_h(T, x_k^h - h^{1/3}), y_d(x_k^h))}{y_h(T, x_k^h + h^{1/3}) - y_h(T, x_k^h - h^{1/3})}$$

Next let  $\omega \in C_c^{0,1}((-2,2))$  with  $0 \le \omega \le 1$ ,  $\omega_{[-1,1]} \equiv 1$  be a weighting function and approximate for r > 0 with  $r < \min_{1 \le k < K} |x_{k+1}^h - x_k^h|/8$  the end data (2.13) by

(3.23) 
$$p_i^{N_T,r} = \omega((x_i - x_k^h)/r)p_{x_k^h}^T + (1 - \omega((x_i - x_k^h)/r))\gamma_i\partial_y\psi(y_i^{N_T}, y_{d,i}), \ i \in \mathbb{Z}.$$

We have the following result [79].

THEOREM 3.5. Consider the scheme (3.14) with end data (3.23). Assume that assumptions (H4), (H5) hold. Then there exists a piecewise constant function r(h) > 0

with  $r(h) \to 0$  as  $h \to 0$  such that with the choice r = r(h) in (3.23) the solution of the adjoint scheme (3.14), (3.23) satisfies

 $p_h \to p$  in  $C([0,T]; L^1_{loc}(\mathbb{R}))$  and boundedly everywhere on  $\mathbb{R}^{cl}_T \setminus R_{\varepsilon}$  as  $h \to 0$ 

for all  $\varepsilon > 0$  with the unique reversible solution p of the adjoint equation (2.11), (2.13).

Remark 3.6. For the simplified case of a piecewise constant state  $y_h$  with one stationary shock it is shown in [79] that for the adjoint EO-scheme Theorem 7 holds with  $r(h) = O(h^{\rho})$  for any  $\rho \in [1/3, 1/2)$ .

It should be possible to show this generally by using Theorem 3.4 together with the monotonicity of the adjoint scheme under assumption (H4).

In [53] higher order strong stability preserving (SSP) total variation diminishing Runge-Kutta (TVD-RK) schemes for the time discretization have been considered. It is shown that providing an SSP state scheme is enough to ensure stability of the discrete adjoint. However requiring SSP for both discrete state and adjoint is too strong. Also order conditions for the corresponding discrete adjoint are derived.

An extension of the presented results in this subsection to boundary control problems has recently been established in [80].

A numerical analysis of general finite-difference schemes for homogeneous transport equations leading to reversible solutions is given in [47]. Consistency with the continuous solutions and their relation to duality solutions of the associated forward problem is shown.

A numerical analysis in the scalar case but for problems with large–time optimal control is given in [2, 61] where in particular the long–time effect of spurious numerical viscosity is analysed.

**3.3.** Higher–Order Finite–Volume and Lagragian Schemes. For a solution to problem (1.1) numerical methods [56, 55, 25] have been proposed by iteratively solving (1.2), (2.11)–(2.12) and equation (2.10), respectively. In [56, 55] a central upwind scheme of second–order has been proposed to numerically discretize (1.2) for the scalar and the systems case. More precisely, in the scalar case, the semi–discrete formulation of (3.3) for the evolution of the cell–averages  $y_i$  reads

(3.24) 
$$\frac{d}{dt}y_i = -\lambda\Delta^- F_{i+\frac{1}{2}}, \ y_i(0) = u_i, \ i \in \mathbb{Z},$$

 $\lambda = \Delta t / \Delta x$ , and the flux  $F_{i+\frac{1}{2}}$  is given by

$$(3.25) F_{i+\frac{1}{2}} = \frac{a_{i+\frac{1}{2}}^+ f(y_i^E) - a_{i+\frac{1}{2}}^+ f(y_{i+1}^W)}{a_{i+\frac{1}{2}}^+ - a_{i+\frac{1}{2}}^-} + \frac{a_{i+\frac{1}{2}}^+ a_{i+\frac{1}{2}}^-}{a_{i+\frac{1}{2}}^+ - a_{i+\frac{1}{2}}^-} \left(y_{i+1}^W - y_i^E\right),$$

where the one-sided local speeds are given by

$$\begin{split} a^+_{i+\frac{1}{2}} &= \max \Big\{ \max_{y \in [\min\{y^E_i, y^W_{i+1}\}, \max\{y^E_i, y^W_{i+1}\}]} \{f'(y)\}, 0 \Big\}, \\ a^-_{i+\frac{1}{2}} &= \min \Big\{ \min_{y \in [\min\{y^E_i, y^W_{i+1}\}, \max\{y^E_i, y^W_{i+1}\}]} \{f'(y)\}, 0 \Big\}. \end{split}$$

The values  $y_i^{E,W}$  are the point values of the piecewise linear reconstruction for y on the cell  $C_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$ 

$$y_i^E = y_i + (y_x)_i \frac{\Delta x}{2}, \ y_i^W = y_i - (y_x)_i \frac{\Delta x}{2},$$
  
20

and the numerical derivatives  $(y_x)_i$  are at least first-order approximations to  $y_x(x_i, t)$  obtained using a nonlinear limiter to ensure a non-oscillatory reconstruction. This can be achieved by for example using a minmod limiter [71] for  $\theta \in [1, 2]$ :

$$(y_x)_i = \operatorname{minmod}\left(\theta \frac{y_i - y_{i-1}}{\Delta x}, \frac{y_{i+1} - y_{i-1}}{\Delta x}, \theta \frac{y_{i+1} - y_i}{\Delta x}\right).$$

For the temporal discretization of (3.24) a third–order strong–stability preserving Runge–Kutta method is used, see [49] and also [53]. A first–order HLL method is obtained when using an explicit Euler discretization in time and the following reconstruction and estimate of the local speeds, respectively:

$$y_i^E = y_i^W = y_i$$
 and  $a_{i+\frac{1}{2}}^+ = -a_{i+\frac{1}{2}}^- = \max\{|f'(y_i)|, |f'(y_{i+1})|\}.$ 

For this choice, the flux (3.25) reduces to the modified Lax–Friedrichs flux (3.20) for the choice  $\nu = \lambda \max_{i \in \mathbb{Z}} a_{i+\frac{1}{2}}^+$ .

The adjoint equation (2.11) is linear in p with space and time–dependent transport velocity and source term. In the systems case the set of equations are diagonalized. In [25] a Lagrangian scheme has been proposed that propagates the terminal quantity  $p^T$  backwards along the characteristics. The terminal point of the characteristic  $x_i^c$  is  $x_i$  and the speed is given by f'(y). Due to the absence of a source term, the value  $p_i^{N_T}$  is transported backwards along  $(t, x_i^c(t))$ . This leads to the following system for the computation of p:

$$\begin{aligned} \frac{dx_i^c(t)}{dt} &= f'(y(t, x_i^c(t))), \ x_i^c(T) = x_i, \ i \in \mathbb{Z}, \\ \frac{dp_i^c(t)}{dt} &= 0, \ p_i^c(T) = p_i^{N_T}, \ i \in \mathbb{Z}. \end{aligned}$$

The previous system is solved using an explicit Euler equation with time-step  $\Delta t$  and for  $y(t, x_i^c(t)) = y_i^n$  in the case of a piecewise constant reconstruction at time  $t = t^n$ . For CFL number less than  $\frac{1}{2}$  the characteristics emerging at the cell center  $x_i$  of cell  $C_i$  remain inside the cell  $C_i$  within a single time step. This leads to the following discrete scheme

$$(3.26) \quad p_i^n = \begin{pmatrix} p_i^{n+1} & f'(y_j^n) = 0, \\ (1 - \beta_i^n)p_i^{n+1} + \beta_i^n p_{i+1}^{n+1} & f'(y_j^n) > 0, \\ (1 - \gamma_i^n)p_i^{n+1} + \gamma_i^n p_{i-1}^{n+1} & f'(y_i^n) < 0 \end{pmatrix},$$

$$(3.27) \quad \beta_i^n = \lambda \frac{f'(y_i^n)}{1 - \lambda(f'(y_{i+1}^n) - f'(y_i^n))^+}, \ \gamma_i^n = -\lambda \frac{f'(y_j^n)}{1 - \lambda(f'(y_i^n) - f'(y_{i-1}^n))^+},$$

where  $p_i^{N_T}$  is given by equation (3.15). Denote by  $p_h$  the piecewise constant reconstruction  $p_h(t,x) = \sum_{i,n} \chi_{[t^n,t^{n+1}) \times C_i}(t,x) p_i^n$ . The following result holds true, see [25, Appendix A]:

THEOREM 3.7. Assume that  $f \in C^2(\mathbb{R})$  and is strictly convex. Let  $p_T \in C^{0,1}(\mathbb{R})$ , let y fulfill (H4), and let the discretization  $p_h(T, \cdot) = \sum_{i \in \mathbb{Z}} \chi_{C_i} p_i^{N_T}$  of  $p_T$  be consistent, *i.e.*,

$$\|p_h(T,\cdot)\|_{L^{\infty}(\mathbb{R})} \le M_T, \sup_{x \in \mathbb{R}} \left\|\frac{p_h(T,x+\Delta x) - p_h(T,x)}{\Delta x}\right\| \le L_T.$$

Furthermore, we assume that  $p_h(T, \cdot)$  converges locally uniformly on [-R, R] for  $h \to 0$  and that the CFL condition holds:

$$\lambda \max_{i \in \mathbb{Z}} \{ |f'(y_i^n)| \} \le \frac{1}{4}$$

Then, the discrete approximation  $p_h$  converges on  $\mathbb{R}_T \setminus R_{\epsilon}$  for all  $\epsilon > 0$  locally uniformly to the unique reversible solution  $p \in B(\mathbb{R}_T) \cap C^{0,1}(\mathbb{R}_T \setminus R_{\epsilon})$  in the sense of Definition 2.4 for  $h \to 0$ .

Furthermore, for smooth objectives convergence towards the gradient of J is established, see [25, Theorem A.2]. The problem (1.1) may also be formulated in multiple spatial dimensions. In this case, only formal computations are available. Neglecting the equations for variations in the shock location  $x_i$ , the resulting formal optimality system has been derived in [25] for dynamics in two spatial dimensions. A discretization of the corresponding forward equation (1.2) using a multi-d extension of the previously shown second-order central Upwind scheme has been proposed. This is combined with a numerical integration using a multi-d Lagrangian formulation for the adjoint equation. Numerical results also in the multi-dimensional case on tracking type cost functionals are reported. Further, in order to decrease the total variation on the numerical approximation of the control u obtained by solving (2.10), a nonlinear filtering has been proposed in [55] similar to [40]. Numerical results on the optimal control of isothermal gas dynamics as well as Euler equations have been reported. Further results in the case of Burgers' equation but in the presence of shocks are given in [67].

**3.4. Relaxation Schemes.** Numerical methods based on relaxation have been introduced [63] and rigorously analysed e.g. [13]. Due to their linear transport structure, the tangent vector calculus severely simplifies and this fact has been exploited in [57, 5] to develop a numerical method. For simplicity, we consider only the Jin–Xin relaxation in the case n = 1 and in the case  $g \equiv 0$ . Then, the hyperbolic relaxation to (1.2) is given by a system for  $Y = (Y^{(1)}, Y^{(2)}) = (y, Y^{(2)})$  with

(3.28) 
$$\partial_t Y + \begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix} \partial_x Y = \begin{pmatrix} 0 \\ \frac{1}{\epsilon} (f(Y^{(1)}) - Y^{(2)}) \end{pmatrix}, \ Y(0, x) = \begin{pmatrix} u(x) \\ f(u(x)) \end{pmatrix},$$

and positive parameters  $\epsilon > 0$  and a a > 0, such that the sub characteristic condition [63] holds. If  $u \in L^{\infty}(\mathbb{R})$  and has small total variation, the sequence  $Y^{(1),\epsilon}$  converges in  $L^1_{loc}(\mathbb{R})$  towards a weak solution to equation (1.2), see [13, Theorem 1.2]. For nonnegative and fixed  $\epsilon > 0$  the following result shows the differentiability of the flow generated by the relaxation system [57, Lemma 2.1 and Lemma 2.3]:

THEOREM 3.8. Let  $Y(\cdot, \cdot)$  be a piecewise Lipschitz continuous solution to (3.28) for some  $\epsilon > 0$ . Let the initial data  $Y(0, \cdot) = \bar{Y}$  be piecewise Lipschitz with N simple discontinuities. Let  $(\bar{V}, \bar{\xi}) \in T_{\bar{Y}}$  be a tangent vector to  $\bar{Y}$  generated by the regular variation  $\gamma$  with  $\gamma(\delta) = \bar{Y}_{\delta}$  for  $\delta > 0$ . Let  $Y_{\delta}$  be the solution to (3.28) and initial data  $Y_{\delta}(0, \cdot) = \bar{Y}_{\delta}$ . Then there exists a time  $t_0 > 0$  such that for all  $t \in [0, t_0]$  the path  $\bar{\gamma}$  with  $\bar{\gamma}(\delta) = Y_{\delta}(t, \cdot)$  is a regular variation of  $Y(t, \cdot)$  generating the tangent vector  $(V(t), \xi(t)) \in T_{Y(t, \cdot)}$ . Further,  $(V, \xi)$  is the unique broad solution to

$$V(0, \cdot) = \bar{V}, \ V_t + \begin{pmatrix} 0 & 1\\ a^2 & 0 \end{pmatrix} V_x = \begin{pmatrix} 0\\ \frac{1}{\epsilon} (f'(Y^{(1)})V^{(1)} - V^{(2)}) \end{pmatrix}$$
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outside of the discontinuities of Y. For i = 1, ..., N and along each line of discontinuity  $x_i(t)$  where Y has a discontinuity in the  $k_i$ th characteristic family, it holds

(3.29) 
$$\xi_i(t) = \bar{\xi}_i, \ \langle \ell_j, [V(t, x_i(t))] + [Y_x(t, x_i(t))] \ \xi_i(t) \rangle = 0, \ j \neq k_i,$$

where  $\ell_j$  is the *j*th left eigenvector to the matrix  $\begin{pmatrix} 0 & 1 \\ a^2 & 0 \end{pmatrix}$ . Furthermore, for  $J^*(Y) = J(Y^{(1)})$  given by (1.3) the variation with respect to a tangent vector  $(V,\xi)$  is given by

$$D_u J^*(Y(u)) = \int_{\mathbb{R}} j(x)(V^{(1)})(T, x) \, \mathrm{d}x + \sum_{i=1}^N \left( j(x_i(T)) + j(x_i(T)) \right) \left[ Y^{(1)}(T, x_i(T)) \right] \xi_i(t),$$

where  $j(x) = \gamma(x)\psi'(Y^1(T, x), y_d(x))$ , such that the following expansion holds true

$$J^*(Y_{\delta}) = J^*(Y) + \delta D_u J^*(Y(u)) + o(\delta).$$

Some remarks are in order. The linear transport structure implies that  $\xi_i(t)$  is constant in time and a linear hyperbolic balance equation for V of similar structure as equation (3.28). Further, a descent direction for  $J^*$  can be obtained explicitly for  $Y(T, \cdot) = -(j(\cdot), 0)$  and for  $\xi_i(T)$  accordingly based on the explicit representation of the gradient above.

In [57] a first-order splitting and an Upwind-discretization for the equations for (Y, V) is proposed. For a fixed grid  $\Delta x > 0$  a discretization of  $Y(0, \cdot)$  is proposed fulfilling the transversality condition (2.26), see also [18, Theorem 2.2, Equation (2.18)]. The scheme ensures that this condition remains valid for any positive time. Further results and higher-order schemes are stated in [5]. A particular case is the first-order limiting scheme  $\epsilon = 0$ . In this case, the forward scheme is given by the Rusanov method and the approximation of the solution to the adjoint equation (3.14) is given by

$$p_i^n = \frac{\lambda}{2} f'(y_i^n) \left( p_{i+1}^{n+1} - p_{i-1}^{n+1} \right) + \frac{\lambda}{2} a \left( p_{i+1}^{n+1} + 2\left(\frac{1}{a\lambda} - 1\right) p_i^{n+1} + p_{i-1}^{n+1} \right)$$

with terminal condition (3.15). The following result holds true, see [5].

THEOREM 3.9. Assume f is strictly convex. Consider the fully discrete scheme (3.26) with terminal data (3.15). Assume that  $y_i^n$  are given by a Lax-Friedrich scheme (3.3) and (3.20). Further, assume that a > 0 is such that the subcharacteristic condition

$$\max_{y \in \mathbb{R}} |f'(y)| \le a,$$

holds true. Then, the scheme (3.26) is monotone.

If  $\lambda a \leq \frac{1}{2}$ , then  $p_h$  converges on  $\mathbb{R}_T \setminus R_{\epsilon}$  for all  $\epsilon > 0$  locally uniformly to the unique reversible solution  $p \in B(\mathbb{R}_T) \cap C^{0,1}(\mathbb{R}_T \setminus R_{\epsilon})$  of the adjoint equation (2.11) with terminal data (2.13).

**3.5. Wave–Front Tracking Schemes.** In the systems case, the existence of a solution to the sensitivity equation for y with respect to  $w \in W_{ad}$  is proven using the wave–front tracking algorithm [15]. Despite the fact that wave–front tracking or

front-tracking [58] has been used as a numerical scheme for equation (1.2), so far, only a few results on the application of those methods for the numerical integration of  $\delta y$  or p exist.

In [52] the wave-front-tracking method for equation (1.2) with  $g \equiv 0$ , n = 1 and f piecewise linear and Lipschitz continuous on [-M, M] for some M > 0 (but not necessarily convex) is considered. The control is also piecewise constant with values in [-M, M] and a single discontinuity at  $x = x_1$ . The solution y = y(t, x) to equation (1.2) is piecewise constant and the Rankine-Hugoniot condition holds at each point of discontinuity. For variations in u but not in  $x_1$  it has been shown that y allows for a first order Taylor-expansion in  $L^1_{loc}$  with an explicit formula for  $\delta y$ , see [52, Theorem 7.1]. Also, differentiability of J has been established [52, Theorem 7.1] and some numerical examples of the calculus have been presented.

In [38] the differential structure for piecewise constant controls u and a piecewise linear, monotone flux  $f(y) = \min\{C_1y, C_2\}$  for some constants  $C_i, i = 1, 2$  coupled to a set of finitely many ordinary differential equations has been studied. Here, it has been exploited that if  $y_0$  is piecewise constant with a number of  $1/\Delta x$  discontinuities, the solution in y remains piecewise constant and the shifts in the discontinuities  $x_i$  are constant in time. Explicit computations for the sensitivities  $\delta y$  and  $\delta x_i$  are possible and detailed convergence results for  $\Delta x \to 0$  are available [38, Theorem 2]. This calculus explicitly computes the tangent vectors for wave-front-tracking in case of a (very) particular flux function f and space of controls.

In [70, 16] wave-front-tracking approximation has been used to characterize the attainable set of nonlinear hyperbolic balance laws. Hence, in the case of tracking-type functionals those results provide also optimal controls without necessarily constructing a differential calculus. Those controllability type results will not be investigated further at this point.

**3.6.** Automatic Differentiation. For many existing numerical simulation codes automatic or algorithmic differentiation (AD) is a possibility to obtain sensitivity information [50, 73]. However, black-box application of those AD software tools, like e.g. www.autodiff.org, towards a finite-volume or discontinuous Galerkin code require at least directional differentiability of the solution to state mapping  $u \to y$ . In order to obtain an algorithmic framework that allows for a numerical computation using AD in the context of hyperbolic balance laws, it is required, in particular, to augment a possible numerical simulation code for equation (1.2) by an equation that allows to have the variations with respect to  $w \in W$ .

This augmentation has been followed in several publications [54, 8, 22] based on the following result [54, Lemma 2.8].

THEOREM 3.10. Assume  $y \in Y$  is a weak solution to equation (1.2) for  $u \in U$  such that it has a shock discontinuity across  $(t, x(t)), t \geq 0$ , and the Rankine– Hugoniot condition holds true:

(3.30) 
$$x'(t)[y(t, x(t))] = [f(y(t, x(t)))],$$

where [u(t,x)] = u(t,x+) - u(t,x-). Consider a perturbation of the shock position as  $x^{\epsilon}(t) = x(t) + \epsilon \nu(t)$  for some function  $\nu$ . Then, linearization of (3.30) yields that  $\nu = \xi$  pointwise in t up to  $O(\epsilon^2)$ , where  $\xi(t)$  is a part of the tangent vector  $(v(t, \cdot), \xi(t))$ generated by a regular variation  $\gamma(\epsilon) = y^{\epsilon}$  and where  $\xi$  fulfills equation (2.27).

In [54, 22] this connection has been exploited by augmenting forward numerical schemes by condition (3.30) prior to applying a (customized) AD. In [54] this approach

has been applied to a state–of–the–art computational fluid flow solver and problems of the Burgers' equation and the Euler equations. The correct sensitivities has been correctly numerically computed, whereas the application of black-box algorithmic differentiation fails. For the scalar case and under an one-sided Lipschitz assumption on the jump discontinuities, a descent method based on the differentiation of equation (3.30) has been proposed in [22]. Therein, also  $\Gamma$ –convergence of the discrete states has been proven. The formal concept has also been extended to the multi-dimensional case in [8].

4. Outlook. In this review, we have collected a variety of results reflecting the state of the art in theory and numerical approximation of optimal control problems for scalar and systems of hyperbolic balance laws. Here, our focus was on a variational calculus for discontinuous solutions and convergent discretizations in one spatial dimension. While significant progress has been achieved for the case of strictly convex scalar equations in the last decade, many open problems remain for nonconvex scalar equations, systems and problems in several space dimensions. For the case of systems, so far mainly directional variations are considered, while Fréchet-type differentiability results would be desirable for optimization methods. Moreover, in the case of systems a rigorous sensitivity and adjoint calculus is so far usually based on including the shock curves as state variables, which leads to explicit interior boundary conditions for the adjoint. In particular, this is inconvenient for design and convergence analysis of numerical sensitivity and adjoint schemes. Hence, it would be desirable to have - similar to the scalar case - a convenient characterization of reversible solutions for the adjoint equation that allow the construction and analysis of convergent adjoint schemes without imposing explicit interior boundary conditions. Moreover, the development of convergent discretizations of higher order and the treatment of optimal control problems in several space dimensions poses many open problems for future research regarding, for example, the resolution along multi-dimensional shock curves or the stability of corresponding high-order numerical schemes for sensitivity and adjoint equations.

While the focus of this survey paper was on the optimal control of a single hyperbolic PDE, also networks of hyperbolic conservation laws play an important role, e.g., for the modelling of gas and water networks, communication networks and vehicular traffic networks, see for example [21, 4, 27, 68]. Here, the control enters in the coupling conditions rendering them nontrivial and the development of a variational calculus as well as of convergent sensitivity and adjoint schemes poses additional challenges.

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