An Accurate Deterministic Projection Method for Hyperbolic Systems with Stiff Source Term

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1 Introduction

We study numerical methods for one-dimensional hyperbolic systems of balance laws ($x \in \mathbb{R}; u \in \mathbb{R}^N, N \geq 1$) with very stiff source terms:

$$u_t + f(u)_x = \frac{1}{\varepsilon} S(u), \qquad 0 < \varepsilon << 1. \tag{1}$$

In particular, we are interested in an inviscid, compressible, reacting flow, described by the reactive Euler equations:

$$\begin{pmatrix} \rho \\ \rho u \\ E \\ \rho z \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \\ \rho u z \end{pmatrix}_x = \frac{1}{\varepsilon} \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\rho z K(\tau) \end{pmatrix}. \tag{2}$$

Here, the dependent variables ρ, u, E, and z are the density, velocity, total energy, and the fraction of unburnt gas, respectively. The pressure is given by the following equation of state (EOS),

$$p = (\gamma - 1) \cdot \Big[E - \frac{\rho u^2}{2} - q_0 \rho z \Big], \tag{3}$$

where the parameter q_0 corresponds to chemical heat release, and $\gamma = \text{Const}$. On the right-hand side of (2), $\tau := p/\rho$ is the temperature and ε is the reaction time. Finally, the Arrhenius kinetics term, [9], is

$$K(\tau) = e^{-\tau_c/\tau}, \tag{4}$$

where τ_c is the ignition temperature.

Typically, chemical reaction time scales are much faster than the fluid dynamical ones. Therefore, in order to fully (numerically) resolve detonation waves, one has to take both temporal (Δt) and spatial (Δx) grid scales to be proportional to ε. This may be extremely computationally expensive, or, in the case of higher spatial dimensions, practically impossible. This is the reason why we are interested in *underresolved* numerical methods, where $\Delta t, \Delta x >> \varepsilon$.

In such a case, the chemical reaction may be considered infinitely fast, and thus the Arrhenius kinetics term, (4), may be replaced with (even stiffer) Heaviside kinetics term, [19],

$$K(\tau) = H(\tau - \tau_c) := \begin{cases} 1, & \text{if } \tau \geq \tau_c, \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

Designing an accurate underresolved numerical method for a very stiff system (2)–(3),(5) or, in general, for the system (1) with a very small ε, is a rather challenging problem. Since the system is stiff, it is natural that one may wish to use an operator splitting (fractional step) method. Then, the step of solving the ODE,

$$u_t = \frac{1}{\varepsilon} S(u),$$

reduces to the projection of the computed solution onto an equilibrium state: $u \mapsto \mathcal{P}u$, where $S(\mathcal{P}u) \equiv 0$, while the corresponding homogeneous system of hyperbolic conservation laws,

$$u_t + f(u)_x = 0, \tag{6}$$

can be solved by any (stable) shock-capturing method.

However, if the so-called *deterministic projection operator* is used, this approach may lead to a spurious weak detonation wave that travels with an *unphysical* propagation speed of one grid cell per time step. This occurs since shock-capturing methods smear shock profiles, and as soon as the unphysical value of the temperature in this numerical shock layer is above the ignition temperature, a certain part of the gas gets burnt prematurely. This peculiar numerical phenomenon was first observed by Colella, Majda and Roytburd [8] in 1986, and since then it has attracted lots of attention (see, e.g., [5, 7, 12, 16, 17]). In order to fix this numerical problem, the ignition temperature was artificially increased in [6], or replaced with uniformly distributed random variable (random projection method by Bao and Jin, [2, 3]). Other, more complicated, but rather successful approaches have been proposed in [10, 13, 18].

In this paper, we introduce an **accurate deterministic projection** (**ADP**) method for balance laws with stiff source terms, which may be considered as a simple and robust alternative to the aforementioned approaches. The key idea is to evolve u according to the homogeneous system (6) (this will guarantee the correct propagation speed!), while using the projected values of $\widetilde{u} := \mathcal{P}u$ only whenever they are required (for example, for computing p in the EOS, (3), when the system (2)–(3),(5) is considered).

The paper is organized as follows. In §2, we introduce the ADP approach for a model scalar problem. In §3, we apply the ADP method to the reactive Euler equations.

2 Scalar Problem

We consider the following scalar hyperbolic balance law with a stiff source term, studied in [16, 2, 4, 11],

$$u_t + f(u)_x = \frac{1}{\varepsilon}(u-\alpha)(1-u^2), \qquad -1 < \alpha < 1, \tag{7}$$

subject to a "prepared", piecewise constant initial data,

$$u(x,0) =: u_0(x) = \begin{cases} 1, & \text{if } x \le x_0, \\ -1, & \text{if } x > x_0. \end{cases} \tag{8}$$

Here, $0 < \varepsilon \le 1$ is a small parameter, f is a convex flux function, and x_0 is a given point. This is a "toy model", where one can easily see the major difficulty we encounter while dealing with hyperbolic problems with stiff source terms.

The source in (7) admits three equilibria: two of them, $u = \pm 1$, are stable, and the third one, $u = \alpha$, is unstable. The exact solution is the shock discontinuity,

$$u(x,t) = \begin{cases} 1, & \text{if } x \le x_0 + st, \\ -1, & \text{if } x > x_0 + st, \end{cases} \tag{9}$$

where the shock speed, determined by the Rankine-Hugoniot condition, is

$$s = \frac{f(1) - f(-1)}{2}. \tag{10}$$

Note that the speed is independent of α, and that the solution of the initial value problem (IVP) (7)–(8) is identical to the solution of the corresponding homogeneous equation,

$$u_t + f(u)_x = 0, \tag{11}$$

with the same initial data (8).

Let us now consider the operator splitting method for the IVP (7)–(8). We denote by $\mathcal{S}_C(\cdot)$ the solution operator, associated with the homogeneous convection equation (11), and by the $\mathcal{S}_R(\cdot)$ the solution operator of the stiff (reaction) ODE,

$$u_t = \frac{1}{\varepsilon}(u-\alpha)(1-u^2). \tag{12}$$

Assume that the solution of (7)–(8) at time level $t = t^n$, $u(x,t^n)$, is given. According to the operator splitting technique, the solution at time $t^{n+1} = t^n + \Delta t$, $u(x,t^{n+1})$, is then approximated by

$$u^{n+1}(x) = \mathcal{S}_R(\Delta t)\mathcal{S}_C(\Delta t)u(x,t^n).$$

In fact, if one uses the exact solution operators, $\mathcal{S}_R$ and $\mathcal{S}_C$, this approximation will be exact, that is $u^{n+1}(x) \equiv u(x,t^{n+1})$.

However, in practice one has to use approximate solution operators instead of the exact ones. Let $\widetilde{\mathcal{S}}_C(\Delta t)$ corresponds to one step of a shock-capturing method. In the studied case of the underresolved numerical method ($\varepsilon << \Delta t$), the second approximate solution operator, $\widetilde{\mathcal{S}}_R(\Delta t)$, will be reduced to the following projection operator:

$$\widetilde{\mathcal{S}}_R(\Delta t)w \equiv \mathcal{P}_\alpha w := \begin{cases} 1, & \text{if } w > \alpha, \\ -1, & \text{if } w \le \alpha, \end{cases} \qquad \forall w \in \mathbb{R}. \tag{13}$$

When $\widetilde{\mathcal{S}}_C(\Delta t)$ is applied to the solution $\left\{u_j^n \approx u(x_j, t^n)\right\}_{j=1}^J$, computed at time t^n, the resulting shock profile, $u^* = \widetilde{\mathcal{S}}_C(\Delta t)u^n$, will be smeared. If the projection operator is applied to u^*, it will result in the following step function (assuming, for simplicity, that the approximate solution operator $\widetilde{\mathcal{S}}_C$ is monotone):

$$u_j^{n+1} = \begin{cases} 1, & \text{if } u_j^* > \alpha, \\ -1, & \text{if } u_j^* \le \alpha, \end{cases} \qquad \forall j.$$

Let us compare $\left\{u_j^n \approx u(x_j, t^{n+1})\right\}_{j=1}^J$ with $\left\{u_j^n \approx u(x_j, t^n)\right\}_{j=1}^J$. Depending on α and on the values of u_j^* in the numerical shock layer, the shock location may be shifted by several grid cells to the right (or to the left), or it may remain at the same location as at time t^n. Next time step of such a *"standard" deterministic projection method* will result in **exactly** the same move of the shock, and so on. As a result, we obtain a shock that propagates with an artificial speed of several cells per time step, which is, in general, not equal to the physically correct speed given by (10).

We propose a very simple ADP method that allows to capture the location of the discontinuity accurately (within the accuracy of a shock-capturing scheme used). Our approach can be schematically presented in the following operator form:

$$u^N = \mathcal{P}_\alpha \widetilde{\mathcal{S}}_C(T)u^0, \tag{14}$$

where $T = N\Delta t$ is a final time, and $\widetilde{\mathcal{S}}_C(T) = \widetilde{\mathcal{S}}_C(\Delta t) \circ \ldots \circ \widetilde{\mathcal{S}}_C(\Delta t) \circ \widetilde{\mathcal{S}}_C(\Delta t)$.

If $\widetilde{\mathcal{S}}_C(\cdot)$ corresponds to a convergent method for the homogeneous IVP (11),(8), then the intermediate solution, $u^* := \widetilde{\mathcal{S}}_C(T)u^0$, will be a (smeared) approximation to the exact solution, (9), where the width of the numerical shock layer is typically of size $\mathcal{O}(\Delta x)$. The projection, $\mathcal{P}_\alpha u^*$, will then result in a step function with a discontinuity, located within $\mathcal{O}(\Delta x)$ from the exact location ($x = x_0 + sT$).

In Figures 1a,b, we present both accurate solutions, computed by the proposed ADP method, (14), and inaccurate solutions, computed by the "standard" deterministic projection method,

$$u^{n+1} = \mathcal{P}_\alpha \widetilde{\mathcal{S}}_C(\Delta t)u^n,$$

with the same approximate solution operator $\widetilde{\mathcal{S}}_C$. In these examples, the flux is $f(u) = u + u^2/2$, and α is taken to be 0.5 and -0.75, respectively. The

initial discontinuity is placed at $x_0 = 0.3$; $\Delta x = 0.02$, $\Delta t = 0.01$, the final time is $T = 0.6$ (60 time steps), the correct shock speed is $1/2$.

These numerical examples clearly demonstrate the accuracy and robustness of the ADP method for the considered scalar problem.

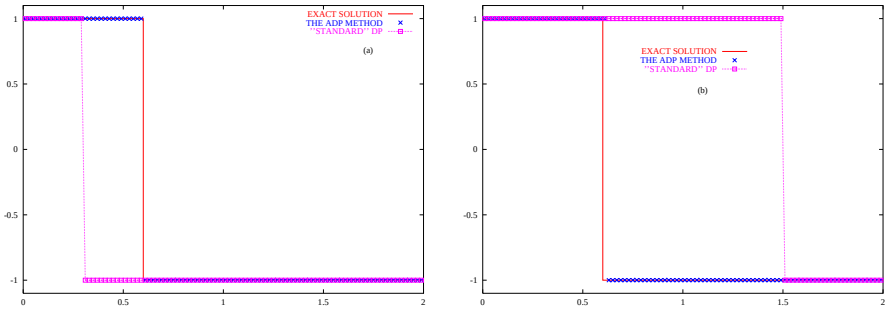

Fig. 1. The solutions of the IVP (7)–(8) with (a) $\alpha = 0.5$, (b) $\alpha = -0.75$

3 Detonation Waves

In this section, we develop the ADP method for the reactive Euler equations. First, note that system (2) can be viewed as the homogeneous system,

$$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{pmatrix}_x = 0, \tag{15}$$

coupled (through the EOS (3)) with the inhomogeneous equation, describing the propagation of the interface between the burnt and unburnt species,

$$(\rho z)_t + (\rho u z)_x = -\frac{1}{\varepsilon} \rho z K(\tau). \tag{16}$$

Thus, when solving system (15)–(16), the operator splitting (and hence, a projection step) should be applied only to equation (16). It is known, [8], that the "standard" projection may lead to spurious, unphysical shock waves traveling with an artificial speed (similarly to the scalar case in §2). Utilizing the ADP method allows one to avoid such an undesirable situation.

3.1 The ADP Method for Stiff Detonation Waves

Unfortunately, the method, described in §2, cannot be applied to the reactive Euler equations straightforwardly, since at every time step we need to

know the projected values of z (which have to be equal to either 0 or 1) for computing p in the EOS (3)). In this case, the accurate projection procedure can be implemented as follows.

Assume that we have computed a solution at time level $t = t^n$. After the convection step, we obtain $\{z_j^*\}_{j=1}^J$, which are then projected by the deterministic projection operator:

$$\widetilde{z}_j^{n+1} = \mathcal{P}_{\tau_c}(z_j^*) := \begin{cases} 1, & \text{if } \tau_j^n \geq \tau_c, \\ 0, & \text{if } \tau_j^n < \tau_c. \end{cases} \tag{17}$$

These values (not the smeared values of z_j^*, computed by the shock-capturing method!) are to be used in the EOS, and thus, for the evolution of $\rho, \rho u$, and E by solving (15). At the same time, in order to avoid appearance of nonphysical waves, the non-projected values,

$$z_j^{n+1} := z_j^*,$$

should be used for the evolution of ρz via the corresponding homogeneous equation,

$$(\rho z)_t + (\rho u z)_x = 0. \tag{18}$$

Remark 1. Note that at every time level we keep two sets of values of z: $\{z_j^n\}_{j=1}^J$ and $\{\widetilde{z}_j^n\}_{j=1}^J$.

Remark 2. The ADP method for the reactive Euler equations resembles the level set method, used in multifluid computations (see, e.g., the review paper [1] and the references therein): we use equation (18) to track the interface between the burnt and unburnt species. However, unlike the multifluid situation, here both z and u are discontinuous at the interface.

Remark 3. In fact, due to the specific structure of the stiff system (15)–(16), the ADP method for the reactive Euler equations can be simplified even further. Note that the values of $z_j^{n+1} \equiv z_j^*$ are used neither in the homogeneous system (15), nor in the EOS (3) that couples system (15) with equation (18). Indeed, one may completely avoid solving equation (18), since the projection, carried out in (17), also does not employ smeared (and thus, unphysical) values of z_j^*. The latter ensures that the computed location of the interface will always be $\mathcal{O}(\Delta x)$ away from the exact one, provided a numerical method, used for solving the homogeneous system (15), converges to its correct entropy solution.

Remark 4. The proposed method can be implemented with one's favorite hyperbolic solver. In the presented numerical examples (both in §2 and §3.2), we have used the second-order central-upwind scheme from [15].

3.2 Numerical Examples

In this section, we demonstrate the performance of the proposed ADP method by applying it in a rather complicated situation, where a detonation wave collides with a shock, a contact discontinuity, and a rarefaction wave. This example is taken from [14, 3].

The parameters are:

$$\gamma = 1.2, \quad q_0 = 50, \quad \tau_c = 3, \quad \frac{1}{\varepsilon} = 230.75.$$

The initial data are:

$$(\rho, u, p, z)(x, 0) = \begin{cases} (\rho_l, u_l, p_l, 0), & \text{if } x \le 10, \\ (\rho_m, u_m, p_m, 1), & \text{if } 10 < x \le 40, \\ (\rho_r, u_r, p_r, 1), & \text{if } x > 40, \end{cases}$$

where $\rho_l = 3.64282, u_l = 6.2489, p_l = 54.8244$; $\rho_m = 1, u_m = 0, p_m = 1$; and $\rho_r = 4, u_r = 0, p_r = 10$. These data correspond to a right moving detonation, a left moving shock, a stationary contact, and a right moving rarefaction. A series of collisions occur after the detonation catches up with the other waves.

We compare the solutions, computed by the ADP method and by the "standard" deterministic projection method. In both cases, we take $\Delta x = 0.125$ and $\Delta t = 0.005$. The reference solution is computed using the fully resolved calculation with $\Delta x = 0.005$ and $\Delta t = 0.00025$.

In Figure 2, we show the computed solutions (density, pressure, temperature, and fraction of unburnt gas) at time $T = 2$ (before collisions). At this time, both methods provide rather accurate approximations.

The results at a later time $T = 4$ (after the collision with the shock, but before the collision with the rarefaction wave) are shown in Figure 3. At this time, only the density is sufficiently accurately captured by the "standard" deterministic projection method, while an unphysical shock wave has already appeared in the other components. At the same time, the location and amplitude of discontinuities, obtained by the ADP method, are correct.

Finally, in Figure 4, we present the results obtained at time $T = 8$ (after all collisions). The computations with the "standard" method are now completely wrong, while the resolution, achieved by the ADP method, is as high as at the smaller times.

Remark 5. We have also tested the ADP method on a variety of examples taken from [2, 3]. The physically correct solutions have been accurately captured in all the performed numerical experiments.

Acknowledgement. The author thanks the participants of the applied and computational mathematics seminar at Tulane University for a number of stimulating discussions. This work was supported in part by the NSF Grant DMS-0073631.

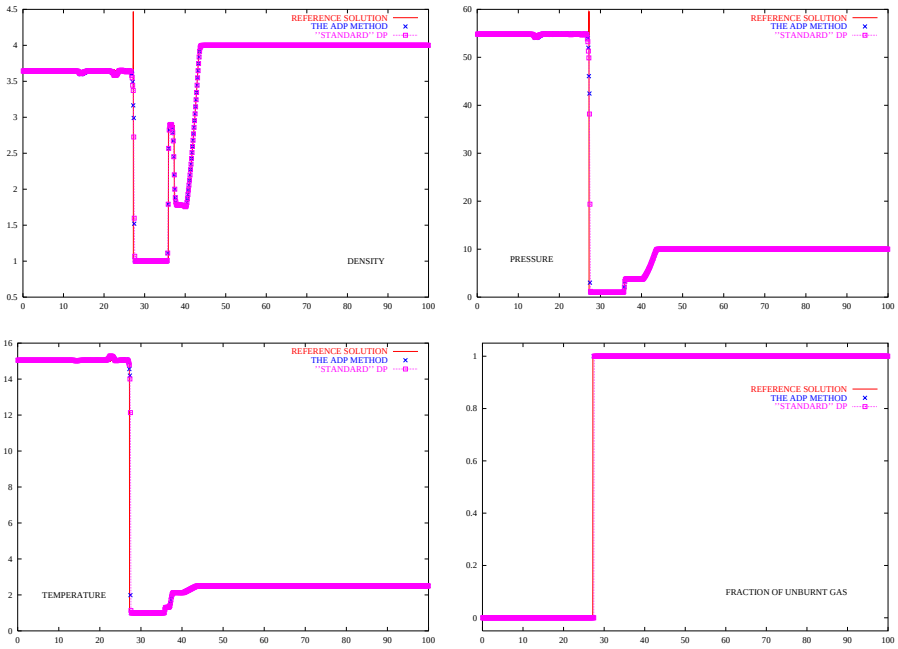

Fig. 2. $T = 2$

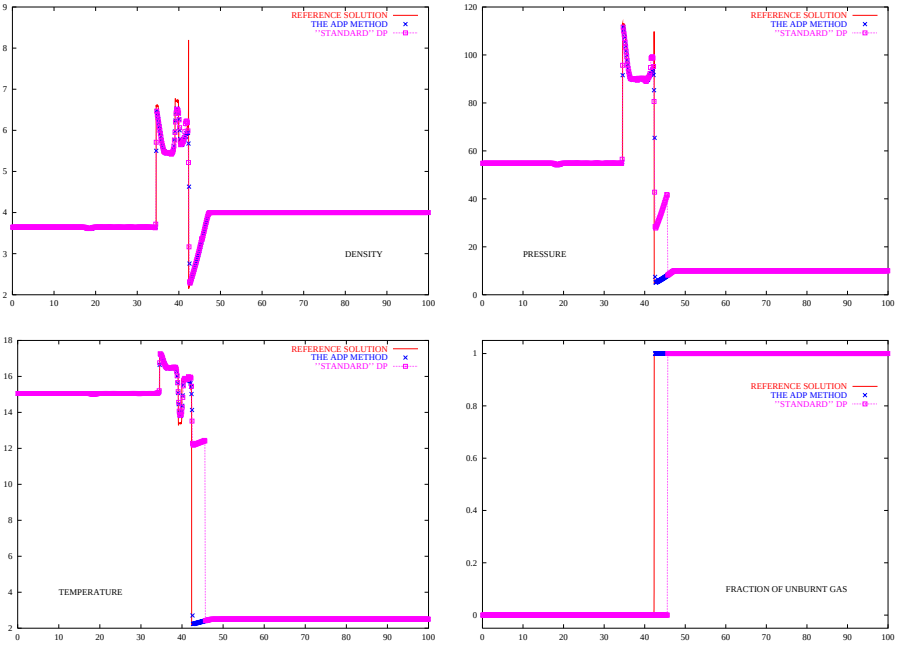

Fig. 3. $T = 4$

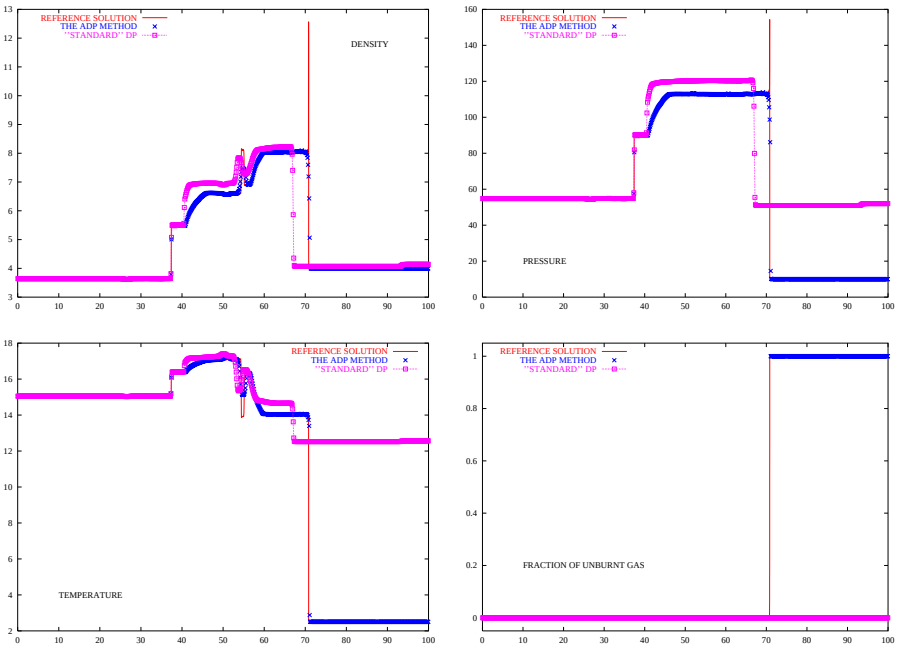

Fig. 4. $T = 8$

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