AN EXPLANATION TO THE PHENOMENON OF COUPLED FIRST ORDER SHIFT OF CONSERVATIVE QUANTITIES DURING THE INTERACTION OF CAPTURED DISCONTINUITIES

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Abstract. High resolution capturing schemes generally speaking can take advantage of the piece-wise smooth property of the weak solutions of conservation laws and achieve high order accuracy wherever the solution is smooth. Thus In 1D, the positions of smeared discontinuities may supposedly be recovered before they interact with each other using the subcell resolution methods (Harten [9]). An interesting phenomenon is that after their interaction, the recovered positions of smeared discontinuities degenerate to first order. We study this phenomena in an ideal model and give an explanation.

Key words. front tracking, Godunov scheme, shock capturing.

AMS subject classifications. 65M60, 65M12

1. Coupled First Order Shift of Conservative Quantities. High resolution capturing schemes take advantage of the piece-wise smooth property of the weak solutions of conservation laws and achieve high order accuracy wherever the solution is smooth. However there are situations in which most high order capturing schemes fail to perform well. In [2], startup errors brought to the numerical solution are investigated. In [15, 16], various difficulties for Godunov type schemes are discussed for computation in elastic-plastic solids. Here we use a few examples to demonstrate some interesting phenomena which could be important for the improvement of capturing schemes.

In the following example we use a 2nd order TVD scheme [8] to compute a Riemann problem for Euler equation for ideal gas with $\gamma = 1.4$. Initially the density, velocity and pressure are $1, 0, 1$ respectively in $(0, 7)$; $\frac{1}{2}, 0, 10$ respectively in $(7, 14)$. With CFL factor equal to 0.95, we measure at the final time $T = 1.4$ the positions of the smeared shock wave and contact using the subcell resolution method (Harten [9]) based on the conservation of mass, see Table 1.1. It is clear from the Table that both the shock and contact positions are only first order accurate.

We also compute the errors for the uniform states away from the shock wave and the contact. They all have second order accuracy, which means the first order shift of conservatived quantities is caused by the coupling between the captured shock and contact. This phenomenon can also happen when two captured discontinuities interact with each other; this will be demonstrated in the next example. When a capturing scheme is used along with interface tracking methods, the accuracy of the captured discontinuity position has a direct connection with the order of accuracy of the tracked interface position because it affects the timing of wave collision and may also affect the accuracy in the smooth parts of the weak solution with non-zero space and time gradients. Therefore modeling this type of interaction seems to be a problem of fundamental importance.

In Table 1.2, there is also the phenomenon of first order shift of conservative quantities when a captured shock hitting a captured contact. Initially the density,

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N	*shock position error*	*order*	*contact position error*	*order*
200	0.028	-	0.016	-
400	0.013	1.1	0.0094	0.77
800	0.0064	1.0	0.0047	1.0
1600	0.0032	1.0	0.0024	0.97

TABLE 1.1
Shock and contact position errors under mesh refinement.

N	*shock position error*	*order*
200	0.016	-
400	0.0086	0.90
800	0.0045	0.93
1600	0.0022	1.0
3200	0.0011	1.0

TABLE 1.2
Reflecting shock position error after interaction with a contact, computed by 2nd order TVD capturing scheme.

velocity and pressure are

$$3.0905645962484498, 1.8445453576892512, 6.0298254275965366$$

on $(0, 8)$; $1, 0, 1$ on $(8, 10)$; $2, 0, 1$ on $(10, 16)$. The right going shock wave initially at $x = 8$ will meet the contact at $x = 10$ and split into reflecting and transmitting shock waves. It is also computed by the second order TVD scheme from time $T = 0$ to time $T = 3$. The reflecting shock wave position is measured using subcell resolution method.

We also measure the captured shock wave position before interacting with the contact to obtain close to second order accuracy.

Is this kind of first order shift of conservative quantities avoidable among the existing capturing methods? Can we develop a high resolution capturing scheme that is at lea st second order in the shift of conservative quantities after captured discontinuities interact? We will try to give a hint of what is happening in the last section.

2. Its Relation to Conservative and Non-Conservative Interface Tracking for Gas Dynamics. The conservative quantity loss across the interface when using a non-conservative tracking methods, e.g. non-conservative front tracking is usually small in 1D when the interface is not interacting with shock waves. But non-conservative and conservative front tracking methods can still be characteristically distinguished in numerical experiments. In [6], we conduct a test for the 1D Euler equation for ideal gas, with $\gamma = 1.4$. The computational domain is $[0, 4]$ with flow-through boundary conditions. At time $T = 0$ there is a central rarefaction wave in $(1, 2)$ and a left going shock at 3. The left going shock runs into the rarefaction wave at the final time $T = 1$. The initial states are as follows: the density, pressure, velocity are $2.0, 0.5, -1.0$ respectively in $(0, 1)$; the pressure is 1.5 in $(2, 3)$; the velocity is -1.5 in $(3, 4)$. The interior capturing scheme is the second order MUSCL scheme [17, 18, 3] with the shock wave tracked conservatively in one case and non-conservatively in the other. The comparative shock position errors are shown in Table 2.1. This demon-

	non-conserv. tracked		*conserv. tracked*	
N	*shock position error*	*order*	*shock position error*	*order*
100	1.52e-5	-	1.26e-4	-
200	5.19e-6	1.55	4.44e-5	1.50
400	-1.80e-6	1.53	1.72e-5	1.37
800	-6.55e-6	-	4.80e-6	1.84
1600	-3.85e-6	0.767	1.26e-6	1.93
3200	-1.92e-6	1.00	3.16e-7	2.00

Table 2.1

Comparative shock position errors for conservative and non-conservative front tracking when interacting with a captured rarefaction wave computed from an initial rarefaction wave fan.

	non-conserv. tracked		*conserv. tracked*	
N	*shock position error*	*order*	*shock position error*	*order*
100	-4.20e-6	-	2.90e-4	-
200	-4.58e-6	-	9.15e-5	1.66
400	-2.54e-5	-	1.71e-5	2.42
800	-2.29e-5	-	2.85e-6	2.58
1600	-1.12e-5	1.03	9.70e-6	1.55
3200	-5.38e-6	1.06	2.00e-7	2.28

Table 2.2

Comparative shock position errors for conservative and non-conservative front tracking when interacting with a captured rarefaction wave computed from an initial smooth rarefaction wave fan.

strates that certain second order information is kept during the interaction of the conservatively tracked shock wave and the rarefaction wave. It is also demonstrated in [6] that if the edges of the initial rarefaction wave is smoothed out, the conservatively tracked shock position will be improved while the non-conservatively tracked one is still first order, see Table 2.2. The next example shows that a conservatively tracked contact will keep its accuracy close to second order when interacting with a captured (by TVD scheme) rarefaction wave.

Initially the density, velocity and pressure are

$$0.3483732641877501, -1.8445453576892512, 6.0298254275965366$$

in $(0, 4)$; $\frac{1}{2}, 0, 10$ in $(6, 8)$; and $1, 0, 10$ in $(8, 16)$. The initial "rarefaction wave" spanning $(4, 6)$ is smoothed out without any sharp corner. Table 2.3 shows the contact position error at the final time $T = 0.8$ when th e contact runs into the rarefaction wave.

But unfortunately this higher order information is lost if we compute the rarefaction wave from an initial discontinuity instead of an initial rarefaction fan. This seems to be related to the startup error [2]. In fact if we change the previous initial data to density, velocity and pressure being

$$0.3483732641877501, -1.8445453576892512, 6.0298254275965366$$

in $(0, 4)$; $\frac{1}{2}, 0, 10$ in $(4, 8)$; $1, 0, 10$ in $(8, 16)$, and compute the conservatively tracked contact position at final time $T = 1$ (so that the contact runs into rarefaction wave), we have essentially first order result in Table 2.4 .

N	*contact position error*	*order*
200	1.5e-04	-
400	1.7e-05	3.1
800	7.3e-06	1.2
1600	2.3e-06	1.7
3200	2.1e-07	3.5

TABLE 2.3
Conservatively tracked contact position errors when interacting with a smooth rarefaction wave.

N	*contact position error*	*order*
200	0.0077	-
400	0.0039	0.98
800	0.0019	1.0
1600	8.7470e-04	1.1
3200	3.7582e-04	1.2

TABLE 2.4
Conservatively tracked contact position errors when interacting with a rarefaction wave computed from an initial discontinuity.

This further emphasizes the close connection between the front tracking method and the high resolution Godunov type interior capturing scheme. In fact they share a highly successful principle, that is, to squeeze as much as possible the high order information from the smooth part of the solution and leave the residue, the discontinuities separating them to the Riemann solvers. That is why we are not too surprised to find out that when a captured shock wave with close to 2nd order accurate position (measured with subcell resolution method) interacts with the conservatively tracked contact, the accuracy of the contact position degenerates to only first order. Because all the high order informations about the shock and the tracked contact are all there before the interaction, we are really curious on what happens during the interaction.

3. An Explanation. Consider a piecewise smooth function u_1

$$u_1(x) = \begin{cases} 2, & x < 3.5 \\ 1, & 3.5 \le x < 6.5 \\ 3, & 6.5 \le x \le 10. \end{cases} \tag{3.1}$$

Let $\{x_i = i : i = 0, 1, \cdots, 10\}$ be a partition on $[0, 10]$ and let $U_1(x)$ be a finite volume approximation of $u_1(x)$. Ideally, we let $U_1(x)$ be the cell average $\frac{1}{x_{i+1}-x_i}\int_{x_i}^{x_{i+1}} u_1(s)ds$ for $x \in (x_i, x_{i+1})$. See Fig. 3. Notice that in this example the positions of discontinuities of $u_1(x)$ can be calculated exactly from its approximation $U_1(x)$ by the subcell resolution method (Harten [9]).

Suppose the two discontinuities of $u_1(x)$ are two approaching shocks. When they all get into one cell, we have a function $u_2(x)$ defined as

$$u_2(x) = \begin{cases} 2, & x < 4.25 \\ 1, & 4.25 \le x < 4.75 \\ 3, & 4.75 \le x \le 10. \end{cases} \tag{3.2}$$

Denote the piecewise cell average of $u_2(x)$ to be $U_2(x)$. See Fig. 3.2. Clearly, the cell average of $u_2(x)$ in cell $(4, 5)$ can not uniquely determine the positions of

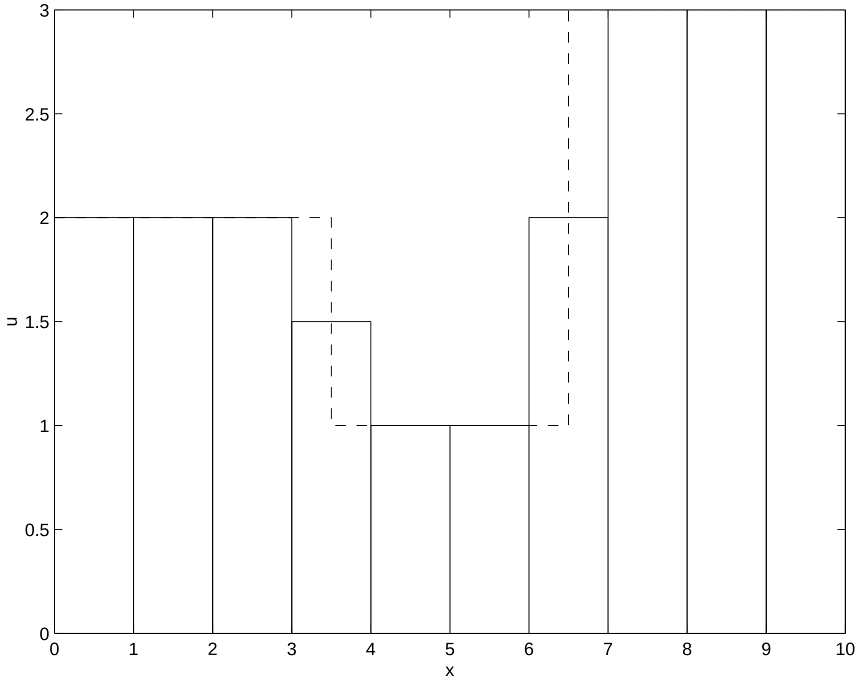

FIG. 3.1. *Discontinuous function* u_1*, "—", and its piecewise average.*

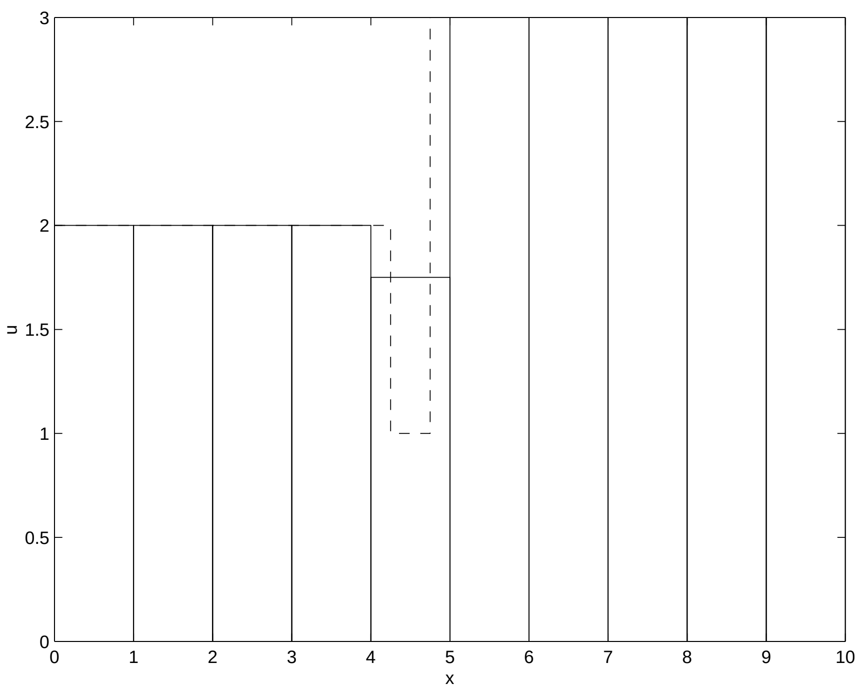

FIG. 3.2. *Discontinuous function* u_2*, "—", and its piecewise average.*

the two discontinuities of $u_2(x)$. In fact, there are infinitely many choices of the two discontinuity positions in cell $(4, 5)$ which give the same cell average in $(4, 5)$. Therefore the order of accuracy of discontinuity positions degenerate to 1 for $U_2(x)$ and any high order information for discontinuity positions of $u_2(x)$ is completely lost in $U_2(x)$. If a numerical evolution scheme starts with $U_2(x)$ as its initial value we can not expect it to achieve more than 1st order accuracy in recovering the discontinuity positions and even in the non-trivial smooth region between the two discontinuities.

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