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N91-21074
p-11

ON THE APPLICATION OF ENO SCHEME WITH SUBCELL RESOLUTION TO CONSERVATION LAWS WITH STIFF SOURCE TERMS

Shih-Hung Chang*
Department of Mathematics, Cleveland State University
Cleveland, Ohio 44115

ABSTRACT

Two approaches are used to extend ENO schemes to treat conservation laws with stiff source terms. One approach is the application of Strang's time-splitting method. Here the basic ENO scheme and Harten's modification using subcell resolution, ENO/SR scheme, are extended this way. The other approach is a direct method and a modification of ENO/SR. Here the technique of ENO reconstruction with subcell resolution is used to locate the discontinuity within a cell and the time evolution is then accomplished by solving the differential equation along characteristics locally and advancing in the characteristic direction. This scheme is denoted ENO/SRCD. All the schemes are tested on the equation of LeVeque and Yee (NASA TM 100075, 1988) modeling reacting flow problems. Numerical results show that these schemes handle this intriguing model problem very well, especially with ENO/SRCD which produces perfect resolution at the discontinuity.

1. INTRODUCTION

Recently, in studying numerical methods for reacting flow problems, LeVeque and Yee (ref.5) considered certain fundamental questions concerning the extension of current finite difference techniques developed for non-reacting flows to reacting flows. Namely, can one: (i) develop stable methods, (ii) obtain "high resolution" results with sharp discontinuities and second order accuracy in smooth regions, and (iii) obtain the correct jumps at the correct locations? They introduced and studied the following one-dimensional scalar conservation law with parameter-dependent source term

$$u_t + u_x = \psi(u), \tag{1}$$

$$\psi(u) = -\mu u \left(u - \frac{1}{2}\right) (u - 1), \tag{2}$$

where μ is a parameter. This equation becomes stiff when the parameter μ is large. Although this linear advection equation with a source term represents only a simple model of reacting flow problems, by studying its numerical solutions one would encounter some of the difficulties sure to occur in solving more realistic models.

*Research was partially supported under Cleveland State University RCAC Grant, Ohio OBOR Grant in the Research Challenge Program, and NASA Space Act Agreement C99066G while the author was in residence at the Institute for Computational Mechanics in Propulsion (ICOMP), NASA Lewis Research Center, Cleveland, Ohio 44135

In their study, two different approaches were used to construct second order accurate numerical methods. One approach was to use a modification of MacCormack's predictor-corrector method for conservation laws (ref.6), together with two TVD-like versions with appropriate limiters (ref.8,9). The other approach was based on the second order accurate Strang's time-splitting method (ref.7). Their numerical tests revealed that stable and second order schemes can be devised by using either of these approaches. However, in studying the ability of these methods in dealing with propagating discontinuities, it was reported that for a certain reasonably fixed mesh and for the very stiff case, all the methods produced solutions that look reasonable and yet are completely wrong, because the discontinuities are in the wrong locations. Their investigation pointed out that the main difficulty is the smearing of the discontinuity in the spatial direction, which in turn introduced a nonequilibrium state into the calculation. To avoid this difficulty, it will be necessary to increase the resolution near the discontinuity, at least for the purpose of evaluating $\psi(u)$.

The purpose of this paper is to show that numerical methods can be devised to overcome the above mentioned difficulties. We will demonstrate this by extending ENO schemes to treat conservation laws with source terms. We will construct numerical schemes which, when applied to Eq.(1), will produce stable solutions with excellent resolutions at the correct locations of discontinuities. We choose to describe the extensions for the following equation

$$u_t + a u_x = \psi(u), \quad a > 0, \quad (3)$$

where the source term $\psi(u)$ arises from the chemistry of the reacting species. It can be handled similarly for $a < 0$.

The basic ENO scheme (ref.4) depends on an essentially non-oscillatory reconstruction procedure. Harten (ref.3) recently modified this procedure using subcell resolution. The notion of subcell resolution is based on the observation that unlike point values, cell averages of a discontinuous piecewise-smooth function contain information about the exact location of the discontinuity within the cell. Using this observation in his study of conservation laws, Harten (ref.3) obtained a modification of the basic ENO scheme, which he denoted ENO/SR, achieving significant improvement in the resolution of contact discontinuities. Basically, when good approximations to the locations of discontinuities inside the cells are obtained, it is then possible to have good reconstruction of the solution at each time step. Here we will also demonstrate that when the information on the location of the discontinuity is used in treating the source term, significant improvement in numerical results can be obtained.

One approach that we use to extend ENO and ENO/SR is the application of Strang's time-splitting method(ref.7), in which one alternates between solving the conservation law without the source term and the ordinary differential equation modeling the chemistry. The other approach is a direct method and a modification of ENO/SR. Here we use the technique of ENO reconstruction with subcell resolution to locate the discontinuity within a cell and then accomplish the time evolution by solving the differential equation along characteristics locally and advancing in the characteristic direction. Since the subcell resolution and the characteristic direction are essential in the design of this scheme, it is denoted ENO/SRCD. In ref.1, ENO/SRCD was originally implemented using the time-splitting method.

In section 2, we will first describe the construction of ENO/SRCD and then the extensions of ENO and ENO/SR schemes for Eq.(3). In section 3, we present the numerical results obtained

from using these schemes on the model problem of LeVeque and Yee (ref.5). A conclusion will be given in section 4.

2. CONSTRUCTION OF THE SCHEMES

We observe that along the characteristic $x = x_0 + at$, the solution to (3) evolves according to the ODE

$$\frac{d}{dt}u(x_0 + at, t) = \psi(u(x_0 + at, t)), \quad (4)$$

with initial data $u(x_0, 0)$. In the scheme ENO/SRCD, this equation will be solved approximately from the time step t_n to t_{n+1} . At t_n , suppose that we have obtained the numerical solution $v^n = \{v_j^n\}$, where v_j^n represents an approximation to \bar{u}_j^n , the cell average of u over $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ at t_n . Then, to obtain v^{n+1} , we use the following steps:

1. Obtain a reconstruction, $R(x; v^n)$, of the solution from the given values v^n .
2. Locate the discontinuity, if any, within each cell using the subcell resolution technique and modify the reconstruction $R(x; v^n)$ to obtain $\hat{R}(x; v^n)$.
3. Advance $\hat{R}(x; v^n)$ via the ODE (4) along the characteristics to the t_{n+1} level and then take cell averages to complete v^{n+1} .

In ENO/SRCD, steps 1 and 2 will follow the ENO reconstruction procedure with subcell resolution of Harten (ref.3). The reconstructed solution function $R(x; v^n)$ here is a piecewise quadratic polynomial obtained by using the primitive function approach. For the sake of completeness, we will describe in straightforward terms the procedures used. For more details and general discussions on reconstruction with subcell resolution, see ref.3.

Step 1. ENO Reconstruction

Over each cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, choose i such that $j - 2 \leq i \leq j$ and minimizes the following:

$$|v_{i+2}^n - 2v_{i+1}^n + v_i^n| = \min \{|v_{k+2}^n - 2v_{k+1}^n + v_k^n| : k = j - 2, j - 1, j\}.$$

Let $R_j(x; v^n)$ denote the reconstructed quadratic polynomial over this cell. Then

$$R_j(x; v^n) = a_j + s_j (x - x_j) + \frac{1}{2} c_j (x - x_j)^2, \quad (5)$$

where

$$\begin{aligned} c_j &= (v_{i+2}^n - 2v_{i+1}^n + v_i^n)/(\Delta x)^2, \\ s_j &= (v_{i+1}^n - v_i^n)/\Delta x + (j - i - \frac{1}{2}) c_j \Delta x, \\ a_j &= v_j^n - c_j (\Delta x)^2/24. \end{aligned} \quad (6)$$

Step 2. Modification by Subcell Resolution

To detect a discontinuity in a cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, we define

$$F_j(z) = \frac{1}{\Delta x} \left[\int_{x_{j-\frac{1}{2}}}^z R_{j-1}(x; v^n) dx + \int_z^{x_{j+\frac{1}{2}}} R_{j+1}(x; v^n) dx \right] - v_j^n. \quad (7)$$

In our numerical experiment, the following criterion is used. If

$$|s_j| > |s_{j-1}|, |s_j| > |s_{j+1}|, \quad \text{and} \quad F_j(x_{j-\frac{1}{2}}) F_j(x_{j+\frac{1}{2}}) \leq 0, \quad (8)$$

we consider that there is a discontinuity at θ_j in this cell satisfying

$$F_j(\theta_j) = 0. \quad (9)$$

The location θ_j can then be approximated by using any standard root-finding method. We simply use the bisection method in our experiment.

Now, if there is a discontinuity inside the cell at θ_j , a modified reconstruction $\hat{R}_j(x; v^n)$ is used, where

$$\hat{R}_j(x; v^n) = \begin{cases} R_{j-1}(x; v^n), & x_{j-\frac{1}{2}} \leq x < \theta_j, \\ R_{j+1}(x; v^n), & \theta_j < x \leq x_{j+\frac{1}{2}}. \end{cases}$$

Otherwise, we use

$$\hat{R}_j(x; v^n) = R_j(x; v^n).$$

Step 3. Time Evolution and Cell Averaging

Consider the case $a \Delta t < \Delta x$ and that there exists a discontinuity at θ_j inside the cell $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$ with

$$\theta_j \leq x_{j+\frac{1}{2}} - a \Delta t,$$

as shown in Figure 1. At the t_n level, $R_{j-1}(x; v^n)$ is used as the solution to the left of θ_j and $R_{j+1}(x; v^n)$ to the right of θ_j . Since the solution to Eq.(3) evolves according to the ODE (4) along characteristics, we can obtain approximate solution values at the t_{n+1} level by solving Eq.(4) and advancing in the characteristic direction. If $w(x, t_{n+1})$ denotes the solution of Eq.(4) at t_{n+1} over $[x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, obtained by using the initial values $R_{j-1}(x; v^n)$ on $[x_{j-\frac{1}{2}} - a \Delta t, \theta_j]$ and $R_{j+1}(x; v^n)$ on $(\theta_j, x_{j+\frac{1}{2}} - a \Delta t]$, the numerical solution v_j^{n+1} is then an approximation to

$$\frac{1}{\Delta x} \int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} w(x, t_{n+1}) dx.$$

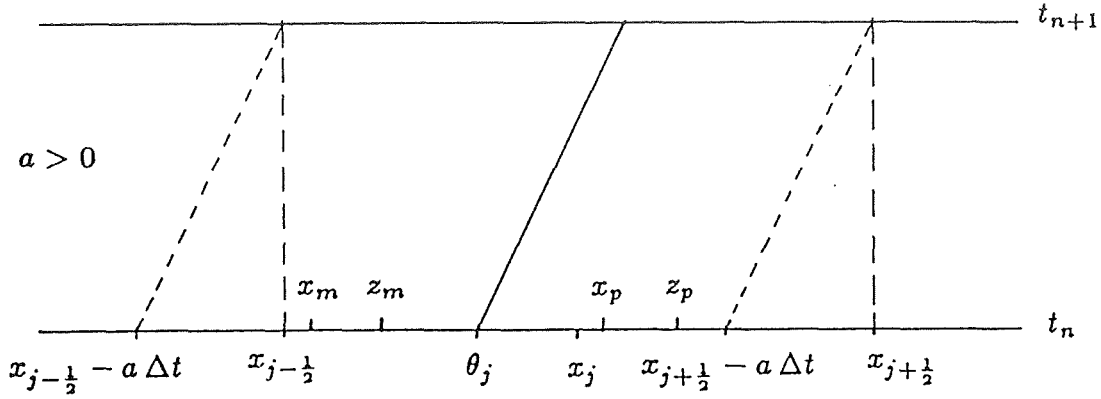


Fig. 1. The case $\theta_j \leq x_{j+\frac{1}{2}} - a \Delta t$

In our present implementation we use the following simple computation. Let x_m and x_p denote the midpoints in the intervals $(x_{j-\frac{1}{2}} - a \Delta t, \theta_j)$ and $(\theta_j, x_{j+\frac{1}{2}} - a \Delta t)$ respectively (see Fig. 1). Then we compute

$$\begin{aligned}
 w_m &= R_{j-1}(x_m; v^n) + \Delta t \psi(R_{j-1}(x_m; v^n)), \\
 w_p &= R_{j+1}(x_p; v^n) + \Delta t \psi(R_{j+1}(x_p; v^n)), \\
 v_j^{n+1} &= [w_m (\theta_j - x_{j-\frac{1}{2}} + a \Delta t) + w_p (x_{j+\frac{1}{2}} - \theta_j - a \Delta t)] / \Delta x.
 \end{aligned} \tag{10}$$

In the above computation, w_m and w_p are obtained from the Euler's method. If the modified Euler method is desired, for example, one simply computes

$$\begin{aligned}
 w_m^* &= R_{j-1}(x_m; v^n) + \Delta t \psi(R_{j-1}(x_m; v^n)), \\
 w_m &= R_{j-1}(x_m; v^n) + \frac{\Delta t}{2} [\psi(R_{j-1}(x_m; v^n)) + \psi(w_m^*)],
 \end{aligned}$$

similarly for w_p^* and w_p , and then v_j^{n+1} by (10). Other locations of θ_j and the cases with regions without discontinuities can be treated similarly and easily. It is quite simple to modify the above scheme to obtain higher order versions.

The extension of ENO and ENO/SR schemes to treat conservation laws with source terms will be done by using Strang's time-splitting method (ref.7). With respect to Eq.(3), the numerical solution v^{n+1} is computed from v^n by

$$v^{n+1} = S_\psi\left(\frac{\Delta t}{2}\right) S_f(\Delta t) S_\psi\left(\frac{\Delta t}{2}\right) v^n, \tag{11}$$

where $S_f(\Delta t)$ represents the numerical solution operator for the conservation law without the source term

$$u_t + a u_x = 0, \quad a > 0, \quad (12)$$

over a time step Δt , and $S_\psi(\frac{\Delta t}{2})$ represents the numerical solution operator for the ordinary differential equation

$$u_t = \psi(u) \quad (13)$$

over $\Delta t/2$. Thus the basic ENO and ENO/SR are used here as the operator $S_f(\Delta t)$. The extended schemes will still be denoted ENO and ENO/SR respectively.

The following second order version of the ENO scheme has been used in ref.2. In our computational experiment, it produces slightly better results than other second order versions.

ENO Scheme:

For the operator $S_f(\Delta t)$, we use

$$S_f(\Delta t) v_j^n = v_j^n - \frac{\Delta t}{\Delta x} (\bar{f}_{j+\frac{1}{2}} - \bar{f}_{j-\frac{1}{2}}), \quad (14)$$

where

$$\begin{aligned} \bar{f}_{j+\frac{1}{2}} = \bar{f}_{j+\frac{1}{2}}^{ENO} = \frac{1}{2} [& f^R(\tilde{v}_j(x_{j+\frac{1}{2}}, t_n), \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_n)) \\ & + f^R(\tilde{v}_j(x_{j+\frac{1}{2}}, t_{n+1}), \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_{n+1}))], \end{aligned} \quad (15)$$

with

$$\begin{aligned} \tilde{v}_j(x_{j+\frac{1}{2}}, t_n) &= v_j^n + \frac{\Delta x}{2} s_j, \\ \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_n) &= v_{j+1}^n - \frac{\Delta x}{2} s_{j+1}, \\ \tilde{v}_j(x_{j+\frac{1}{2}}, t_{n+1}) &= v_j^n + \frac{\Delta x}{2} s_j - \Delta t a s_j, \\ \tilde{v}_{j+1}(x_{j+\frac{1}{2}}, t_{n+1}) &= v_{j+1}^n - \frac{\Delta x}{2} s_{j+1} - \Delta t a s_{j+1}, \end{aligned}$$

where the s_j 's used in the above computation come from (6) in step 1 and $f^R(v_L, v_R)$ denotes the flux at the origin in a Riemann problem with v_L to the left and v_R to the right.

Now, let us describe the operator $S_\psi(\Delta t)$. Here we will follow steps 1 and 2 to find the discontinuity θ_j , if any. Let us use the same notations introduced before and refer to Fig.1. Also, let z_m and z_p denote the midpoints in the intervals $(x_{j-\frac{1}{2}}, \theta_j)$ and $(\theta_j, x_{j+\frac{1}{2}})$ respectively. Then, for approximating cell averages and for the case $\theta_j \leq x_{j+\frac{1}{2}} - a \Delta t$, we use

$$\begin{aligned} S_\psi(\Delta t) v_j^n = v_j^n + \frac{\Delta t}{2 \Delta x} [& \psi(R_{j-1}(z_m; v^n)) (\theta_j - x_{j-\frac{1}{2}}) + \psi(w_m) (\theta_j - x_{j-\frac{1}{2}} + a \Delta t) \\ & + \psi(R_{j+1}(z_p; v^n)) (x_{j+\frac{1}{2}} - \theta_j) + \psi(w_p) (x_{j+\frac{1}{2}} - \theta_j - a \Delta t)], \end{aligned} \quad (16)$$

where w_m and w_p are the same as in (10). Again, other situations are handled similarly.

The resulting algorithm then takes the following form:

$$v_j^{n+1} = S_\psi\left(\frac{\Delta t}{2}\right) S_f(\Delta t) S_\psi\left(\frac{\Delta t}{2}\right) v_j^n. \quad (17)$$

ENO/SR Scheme:

The operator $S_f(\Delta t)$ is now replaced by Harten's second order ENO scheme with subcell resolution (ref.3). It is given in the form of Eq.(14) with

$$\bar{f}_{j+\frac{1}{2}} = \bar{f}_{j+\frac{1}{2}}^{ENO} + \hat{g}_{j+\frac{1}{2}},$$

where $\bar{f}_{j+\frac{1}{2}}^{ENO}$ will be the same as in (15) and the correction term $\hat{g}_{j+\frac{1}{2}}$ is computed as follows. If the discontinuity condition (8) is not satisfied, then

$$\hat{g}_{j+\frac{1}{2}} = \frac{a}{12} (\nu - 1) (2\nu - 1) c_j (\Delta x)^2, \quad \nu = a \Delta t / \Delta x;$$

else

$$\hat{g}_{j+\frac{1}{2}} = \begin{cases} [(\Delta x - a \Delta t) (v_j^n - a \Delta t s_j / 2) - b_{j-1}(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}} - a \Delta t)] / \Delta t, & \text{when } F_j(x_{j+\frac{1}{2}} - a \Delta t) F_j(x_{j-\frac{1}{2}}) > 0, \\ [b_{j+1}(x_{j+\frac{1}{2}} - a \Delta t, x_{j+\frac{1}{2}}) - a \Delta t (v_j^n + (\Delta x - a \Delta t) s_j / 2)] / \Delta t, & \text{otherwise,} \end{cases}$$

and the expression $b_j(y_1, y_2)$ is used to mean

$$b_j(y_1, y_2) = \int_{y_1}^{y_2} R_j(x; v^n) dx.$$

In the above computation, all the c_j 's, s_j 's, and a_j 's come from (6) in step 1. The operator $S_\psi(\Delta t)$ will be the same as in (16) and the final algorithm also takes the same form as in (17).

3. COMPUTATIONAL RESULTS

We use the same fixed mesh and initial data as in the model problem of LeVeque and Yee (ref.5) to test the ability of the above schemes in dealing with propagating discontinuities. Thus, we apply all the schemes to Eq.(1) together with the initial condition

$$u(x, 0) = \begin{cases} 1, & \text{if } x \leq 0.3, \\ 0, & \text{if } x > 0.3. \end{cases}$$

We take $\Delta x = 0.02$, $\Delta t = 0.015$, and the domain in x to be from 0 to 1. For comparison with ref.5, we also show the results at $t = 0.3$ and for the cases $\mu = 1, 10, 100$, and 1000. For all cases, ENO/SRCD produces a perfect resolution as shown in Figure 2. Figure 3 shows the computed results using ENO and ENO/SR schemes for $\mu = 1, 10$, and 100. Here one can see that the

results from ENO/SR are also almost perfect. For the very stiff case, $\mu = 1000$, both ENO and ENO/SR fail to produce stable solutions for the above mesh in our computational experiment. However, when we reduce the size of Δt to one half of the original, i.e., $\Delta t = 0.0075$, and march 40 time steps, very good result is again obtained from ENO and perfect resolution is obtained from ENO/SR as shown in Figures 4a and 4b respectively. We understand that reducing Δt means the reduction of stiffness of the problem. The difficulty arises from the fact that in both ENO and ENO/SR schemes, the computation of the numerical flux $\bar{f}_{j+\frac{1}{2}}^{ENO}$ still produces "large" error in the spatial direction.

The computational results obtained here compare favorably to those in LeVeque and Yee (ref.5).

ENO/SRCD

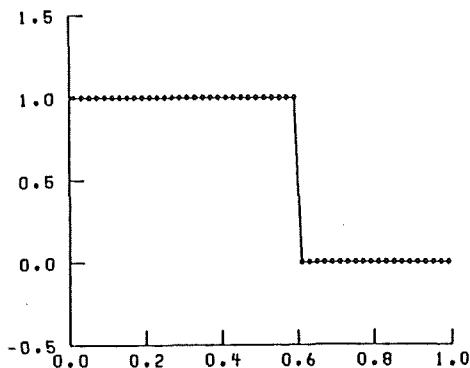


Fig. 2. Numerical results at $t = 0.3$ using ENO/SRCD scheme with discontinuous initial data and $\mu = 1, 10, 100, 1000$. $\Delta x = 0.02, \Delta t = 0.015$, —: true solution, \cdots : computed solution

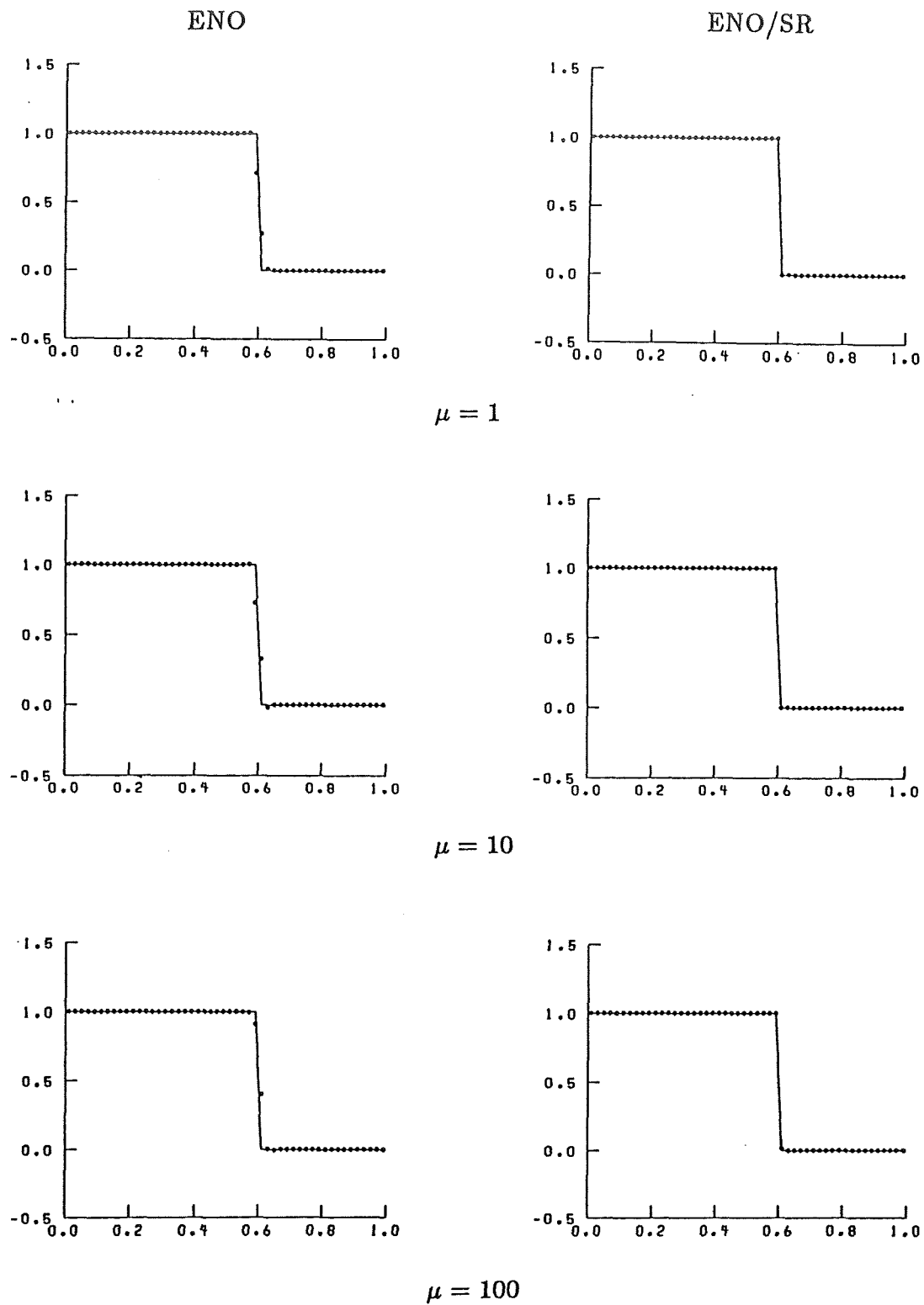


Fig. 3. Numerical results at $t = 0.3$ using ENO (first column) and ENO/SR (second column) schemes with discontinuous initial data for $\mu = 1$ (first row), $\mu = 10$ (second row), and $\mu = 100$ (third row). $\Delta x = 0.02$, $\Delta t = 0.015$, —: true solution, \cdots : computed solution

ENO

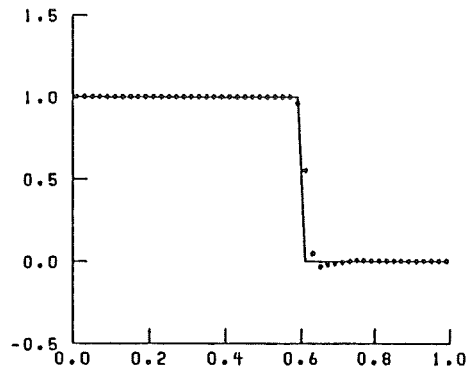


Fig. 4a. Numerical results at $t = 0.3$ using ENO scheme with discontinuous initial data and $\mu = 1000$.
 $\Delta x = 0.02$, $\Delta t = 0.0075$, —: true solution, \cdots : computed solution

ENO/SR

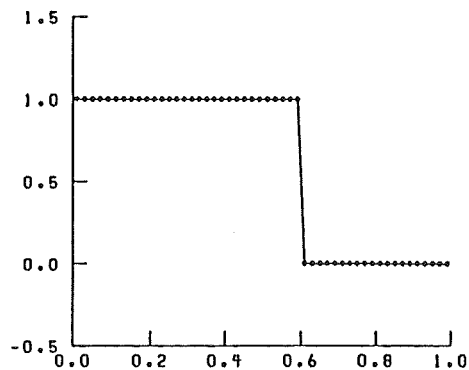


Fig. 4b. Numerical results at $t = 0.3$ using ENO/SR scheme with discontinuous initial data and $\mu = 1000$.
 $\Delta x = 0.02$, $\Delta t = 0.0075$, —: true solution, \cdots : computed solution

4. CONCLUSIONS

We have extended the basic ENO and Harten's ENO/SR schemes to treat conservation laws with source terms. Two approaches are used. One is to apply Strang's time-splitting method, in which one alternates between solving the conservation law without the source term and the ordinary differential equation modeling the chemistry. The other is a modification of ENO/SR and a direct method, which uses the technique of ENO reconstruction with subcell resolution to locate the discontinuity within a cell and then accomplishes the time evolution by solving the differential equation along characteristics locally and advancing in the characteristic direction. We call this scheme ENO/SRCD. All the schemes are tested on the equation of LeVeque and Yee (ref.5) modeling reacting flow problems. The ENO/SRCD scheme produces perfect resolution at the propagating discontinuity. The extensions of basic ENO and ENO/SR via time-splitting also perform very well, especially with ENO/SR showing almost perfect results, except for the very stiff case where some adjustment in the time step-size is needed.

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