# High-order finite difference methods with subcell resolution for hyperbolic conservation laws with stiff reaction terms: preliminary results

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## 1. Motivation and objective

The motivation for this research stems from the high-speed chemical reacting flows which have stiff reaction terms, where the chemical time scales are often much smaller than the fluid dynamics time scales. It is usually too expensive to resolve all the spatial/temporal scales if we are only interested in the main flow. On the other hand, insufficient spatial/temporal resolution will cause the speed of propagation of discontinuities to be incorrectly predicted for many numerical methods. This numerical phenomenon was first observed by Colella *et al.* (1986). Then LeVeque & Yee (1990) showed that a similar spurious propagation phenomenon can be observed even with scalar equations.

Colella *et al.* (1986) and Majda & Roytburd (1990) have successfully applied the random choice method of Chorin (1976, 1977) for the solution of under-resolved detonation waves. However, it is difficult to eliminate completely the numerical viscosity in a shock-capturing scheme. Fractional step methods are commonly used for allowing an under-resolved mesh size with a shock-capturing method. Chang (1989, 1991) applied the subcell resolution method of Harten (1989) to the finite volume ENO method in the convection step, which is able to produce a zero viscosity shock profile in nonreacting flow. The time evolution is advanced along the characteristic line. Correct discontinuity speed was obtained in the one-dimensional scalar case. However, it is difficult to extend this approach to multi-dimensions and to system of equations because of the reliance on the exact time evolution via characteristics. Engquist & Sjögreen (1991) proposed a simple temperature extrapolation method based on finite difference ENO schemes with implicit Runge-Kutta time discretization, which uses a first-/second-order extrapolation of the temperatures from outside the shock profile. The method is easy to extend to multi-dimensions. Their method is not a fractional step method. It does not seem to work well when the spatial scales are under-resolved. Other first-/second-order methods that are based on the fractional step method have been proposed by Bao & Jin (2000, 2001) and Tosatto & Vigevano (2008).

Our objective in this study is to develop a high-order finite difference method which can capture the correct detonation speed in an under-resolved mesh and will maintain high-order accuracy in the smooth part of the flow. The first step of the proposed fractional step method is the convection step which solves the homogeneous hyperbolic conservation law in which any high-resolution shock-capturing method can be used. The aim in this step is to produce a sharp wave front, but some dissipativity is allowed. The second

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step is the reaction step where a modified ODE solver is applied with modified transition points. Here the transition point means the numerical solution in the shock region which is due to the dissipativity of a shock-capturing scheme. Because the transition points in the convection step will result in large erroneous values of the source term if the source term is stiff, we first identify those points and then extrapolate them by a reconstructed polynomial using the idea of Harten's subcell resolution method. Unlike Chang's approach, we apply Harten's subcell resolution in the reaction step. Thus it is flexible to have any shock-capturing scheme as the convection operator. In the reaction step, since the extrapolation is based on the high-order reconstruction, high-order accuracy can be achieved in space. The only drawback in our current approach is that the temporal order will only be, at most, second-order due to the time splitting which is common for most of the previous methods for stiff sources.

## 2. The scalar problem

We first introduce the proposed method for the scalar model problem in LeVeque & Yee (1990), i.e.,

$$u_t + f(u)_x = S(u), \tag{2.1}$$

$$S(u) = -\mu u \left(u - \frac{1}{2}\right)(u-1), \tag{2.2}$$

with the initial condition

$$u(x,0) = \begin{cases} 1, & x \le 0.3 \\ 0, & x > 0.3 \end{cases}. \tag{2.3}$$

The general fractional step approach is as follows. The numerical solution at time level $t_{n+1}$ is approximated by

$$u^{n+1} = R(\Delta t)A(\Delta t)u^n. \tag{2.4}$$

The convection operator $A$ is defined to approximate the solution of the homogeneous part of the problem on the time interval, i.e.,

$$u_t + f(u)_x = 0, \quad t_n \le t \le t_{n+1}. \tag{2.5}$$

The reaction operator $R$ is defined to approximate the solution on a time step of the reaction problem:

$$\frac{du}{dt} = S(u), \quad t_n \le t \le t_{n+1}. \tag{2.6}$$

In the Strang-splitting in Strang (1968), the numerical solution at time step $t_{n+1}$ is computed by

$$u^{n+1} = R\left(\frac{\Delta t}{2}\right) A(\Delta t) R\left(\frac{\Delta t}{2}\right) u^n, \tag{2.7}$$

where the convection operator is over a time step $\Delta t$ and the reaction operator is over $\Delta t/2$. The two half-step reaction operations over adjacent time steps can be combined to save cost.

Next, we introduce the proposed fractional step methods for the convection step and the reaction step separately.

### 2.1. *Convection operator*

Any high-resolution shock-capturing operator can be used in the convection step. The purpose of this step is to minimize the number of transition points in the shock region. In this work, we use the framework of high-order finite difference WENO schemes (Jiang & Shu 1996) with a TVD Runge-Kutta time discretization to solve the one-dimensional conservation law

$$u_t + f(u)_x = 0. \tag{2.8}$$

In particular, for the scalar case, we apply the anti-diffusive flux corrections for the WENO scheme in Xu & Shu (2005) to obtain sharp resolution for contact discontinuities.

### 2.2. *Reaction operator*

If there is no smearing of discontinuities in the convection step, any ODE solver can be used as the reaction operator. However, all the standard shock-capturing schemes will produce a few transition points in the shock when solving the convection equation. These transition points are usually responsible for causing incorrect numerical results in the stiff case. Thus we cannot directly apply the regular ODE solver to these troubled points.

Here we use Harten's subcell resolution technique in the reaction step. The general idea is as follows. If a point is considered a troubled point, i.e., it is a transition point of the shock, its neighboring points which are deemed not troubled will be used instead.

The procedure can be summarized in the following steps:

(1) Use a "shock indicator" to identify cells in which shocks are believed to be situated. Harten proposed the following minmod-based shock indicator. Let

$$s_j = \text{minmod}\{u_{j+1} - u_j, u_j - u_{j-1}\}, \tag{2.9}$$

define the cell $I_j$ as troubled if $|s_j| > |s_{j-1}|$ and $|s_j| > |s_{j+1}|$. Notice that this troubled cell-identifying method will only find the "worst" cell inside a shock transition. That is, if there are several consecutive transition cells, only the worst one will be identified as a troubled cell.

(2) In a shocked cell identified above, we continue to identify its neighboring cells. If the cell $I_{j-s}$ and the cell $I_{j+r}$ $(s, r > 0)$ are the first good cells from the left and the right (i.e., $I_{j-s+1}$ and $I_{j+r-1}$ are still troubled cells), we compute the ENO interpolation polynomial $p_{j-s}(x)$ and $p_{j+r}(x)$ for the cells $I_{j-s}$ and $I_{j+r}$, respectively. Because of the anti-diffusive corrector in the convection step, $r$ and $s$ will not be larger than 2 in general. The modified cell point value $u_j$ is computed by

$$\tilde{u}_j = \begin{cases} p_{j-s}(x_j), & \theta \geq x_j \\ p_{j+r}(x_j), & \theta < x_j \end{cases}, \tag{2.10}$$

where the location $\theta$ is determined by conservation

$$\int_{x_{j-1/2}}^{\theta} p_{j-s}(x)dx + \int_{\theta}^{x_{j+1/2}} p_{j+r}(x)dx = \int_{x_{j-1/2}}^{x_{j+1/2}} u_j dx. \tag{2.11}$$

Under certain conditions, it can be shown that there is a unique $\theta$ satisfying Eq. (2.11), which can be solved using, for example, a Newton's method. If there is no solution for $\theta$ or there is more than one solution, we choose $\tilde{u}_j = u_{j-s}$.

(3) Use $\tilde{u}_j$ instead of $u_j$ in the ODE solver if the cell $I_j$ is a troubled cell.

If an explicit method such as the Euler forward is used, because of the stiffness of the source term, a small CFL number may be required. We shall consider, for example, the

linearized trapezoidal method

$$u_j^{n+1} = u_j^n + \frac{\Delta t S(u_j^n)}{1 - \frac{\Delta t}{2} S'(u_j^n)}. \tag{2.12}$$

Then Eq. (2.12) is modified to

$$u_j^{n+1} = u_j^n + \frac{\Delta t S(\tilde{u}_j)}{1 - \frac{\Delta t}{2} S'(\tilde{u}_j)}, \tag{2.13}$$

if the cell $I_j$ is a troubled cell.

REMARK 1. *For this model problem, we can simplify the above procedure. As indicated above, step (1) only identifies the "worst" cell in the shock transition. In the numerical computation, we simply use its two immediate neighbor cells ($s = r = 1$) for the subcell resolution procedure. This works because the convection operator provides a very sharp shock front.*

REMARK 2. *If a multi-step ODE solver is applied in the reaction step, a modification of the transition points in each step is required.*

### 2.3. *Numerical examples for scalar problems*

In this section, we test the proposed method on three scalar problems. The proposed method uses a fifth-order WENO-Roe scheme (WENO5) with the third-order TVD Runge-Kutta method (RK3) as the convection operator, and a modified ODE solver based on the subcell resolution as the reaction operator. From now on, we use the notation WENO/SR for the proposed WENO scheme. If the anti-diffusive WENO is used in the convection step, the notation anti-diffusive WENO/SR will be used.

#### 2.3.1. *Accuracy test*

We first test the convergence order of the proposed anti-diffusive WENO/SR scheme. We consider Eq. (2.1) with $f(u) = u$ and the source term

$$S(u) = -u + \sin(2\pi(x - t)) \tag{2.14}$$

and periodic boundary conditions on the computation domain $x \in [0, 1]$. The exact solution is $u(x, t) = \sin(2\pi(x - t))$. The errors and orders of accuracy are listed in Table 1. In this smooth problem, there are no troubled cells and thus the anti-diffusive WENO/SR is equivalent to the anti-diffusive WENO scheme. Since both the Strang splitting method and also trapezoidal rule in the reaction step are second-order in time, we set $dt = \text{CFL} \times (dx)^{5/3}$ to achieve the fifth order in space as shown in Table 1.

The next example is to show the ability of the proposed schemes to deal with the propagating shocks.

#### 2.3.2. *A discontinuity example*

This example is the model problem of LeVeque & Yee (1990). Consider Eq. (2.1) with $f(u) = u$ and the initial condition:

$$u(x, 0) = \begin{cases} 1, & x \le 0.3 \\ 0, & x > 0.3 \end{cases}. \tag{2.15}$$

TABLE 1. $L^1$ errors and orders of accuracy by the anti-diffusive WENO5/SR at $t = 0.3$ with CFL=0.6.

| N | error | order |
|---|---|---|
| 10 | 1.02E-02 | – |
| 20 | 4.06E-04 | 4.65 |
| 40 | 1.21E-05 | 5.07 |
| 80 | 3.71E-07 | 5.03 |
| 160 | 1.18E-08 | 4.98 |

For this initial value problem, the exact solution is

$$u(x,t) = \begin{cases} 1, & x \le t + 0.3 \\ 0, & x > t + 0.3 \end{cases} . \tag{2.16}$$

Analytically, the source term should be always zero. However, if $\mu$ in the source term Eq. (2.2) is very large, the numerical errors of $u$ in the transition region can result in large erroneous values of $S(u)$, which must be corrected.

We compare the numerical results by the anti-diffusive WENO5/SR and regular WENO5 schemes in Figure 1 and Figure 2, respectively. For each scheme, we test for the cases of $\mu = 10$, $\mu = 800$ and $\mu = 10000$ with the same mesh $N = 50$ at a final time $t = 0.3$. In the case of $\mu = 10$, both schemes can capture the discontinuity at the correct position (see the left subplots of Figures 1 and 2). For the stiffer case where $\mu = 800$, the propagation speed of the discontinuity computed by regular WENO5 is qualitatively slower than the analytical value as shown by the middle subplot of Figures 2, whereas at $\mu = 10000$, the discontinuity solved by regular WENO5 does not move at all. If the mesh is sufficiently refined, the regular WENO5 can capture the correct solution. However, for this example in the case where $\mu = 10000$, at least $N = 3000$ points are needed.

We remark that in general, the anti-diffusive WENO scheme can capture the discontinuity sharply which usually has, at most, two transition points inside the discontinuity. Thus it does help for the stiff source term problems. For example, for the same stiffness (i.e., same $\mu$), the anti-diffusive WENO requires far fewer points than the regular WENO scheme to resolve the solution. However, if the source term is extremely stiff, even one transition point may cause a wrong discontinuity speed, for which the proposed WENO/SR is needed.

## 3. One-dimensional detonation waves

In this section, we extend our approach to reactive Euler equations. Consider the simplest one-dimensional reactive Euler equation with only two chemical states: burnt gas and unburnt gas. The unburnt gas is converted to burnt gas via a single irreversible reaction. Without heat conduction and viscosity, the equation can be written as

$$\rho_t + (\rho u)_x = 0 \tag{3.1}$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0 \tag{3.2}$$

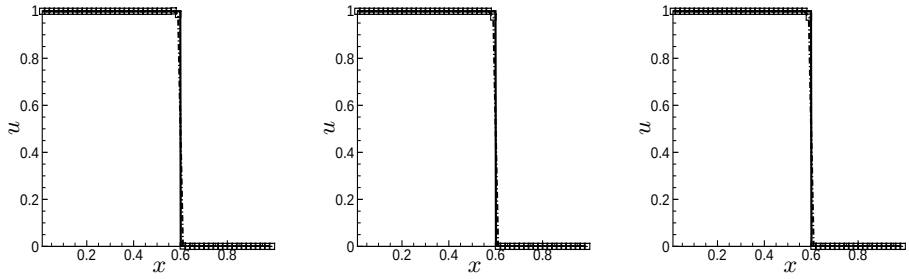


FIGURE 1. Results with the initial condition Eq. (2.15) by the anti-diffusive WENO/SR with $N = 50$. Solid line: exact solution; dashed line with symbols: computed solutions. Left: $\mu = 10$, CFL=0.1; Middle: $\mu = 800$, CFL=0.1; Right: $\mu = 10000$, CFL=0.1.

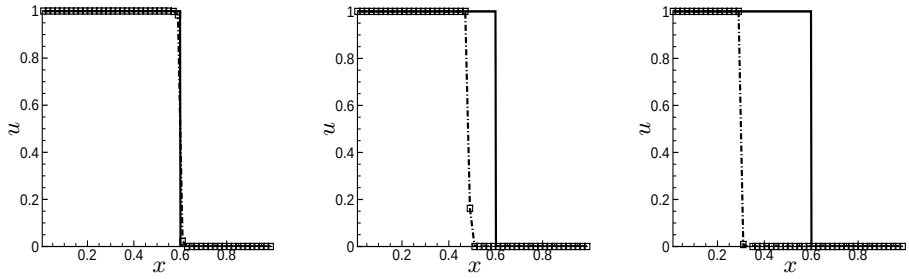


FIGURE 2. Results with the initial condition Eq. (2.15) by the regular WENO scheme with $N = 50$. Solid line: exact solution; dashed line with symbols: computed solutions. Left: $\mu = 10$, CFL=0.1; Middle: $\mu = 800$, CFL=0.1; Right: $\mu = 10000$, CFL=0.05.

$$E_t + (u(E+p))_x = 0 \tag{3.3}$$

$$(\rho z)_t + (\rho u z)_x = -K(T)\rho z, \tag{3.4}$$

where $\rho$ is the mixture density, $u$ is the mixture velocity, $E$ is the mixture total energy per unit volume, $p$ is the pressure, $z$ is the mass fraction of the unburnt gas, $K$ is the chemical reaction rate and $T$ is the temperature. The pressure is given by

$$p = (\gamma - 1)(E - \frac{1}{2}\rho u^2 - q_0 \rho z), \tag{3.5}$$

where $q_0$ is the chemical heat released in the reaction. The temperature is defined as

$$T = \frac{p}{\rho}. \tag{3.6}$$

The reaction rate $K(T)$ is modeled by an Arrhenius law

$$K(T) = K_0 \exp\left(\frac{-T_{ign}}{T}\right), \tag{3.7}$$

where $K_0$ is the reaction rate constant and $T_{ign}$ is the ignition temperature. The reaction rate may be also modeled in Heaviside form

$$K(T) = \begin{cases} 1/\varepsilon & T \geq T_{ign} \\ 0 & T < T_{ign} \end{cases}, \tag{3.8}$$

where $\varepsilon$ is the reaction time and $1/\varepsilon$ is roughly equal to $K_0$.

Now, we apply the similar WENO/SR approach to the one-dimensional system case.

### 3.1. *Convection operator*

In the scalar problem Eq. (2.1), we have applied the anti-diffusive WENO scheme as the convection operator because the discontinuous wave is a contact discontinuity. However, the Chapman-Jouguet (C-J) detonation wave is a shock followed by a reaction. In general, it is not safe to apply the anti-diffusive technique to a shock, since it may generate an entropy-violating solution. Therefore, we do not apply the anti-diffusive sharping procedure here. This is not a problem because the fifth-order WENO scheme is already able to capture the shock very sharply (better than its capability in capturing contact discontinuities). In this section, we use WENO5 with RK3 as the convection operator in the reactive Euler problems.

### 3.2. *Reaction operator*

The reaction step for the system case is slightly different from the scalar case because there are more component variables where $\rho z$ and $T$ are involved in the source term. The key point here is to identify the troubled cell correctly and to extrapolate the variables $\rho z$ and $T$.

(1) To apply the step (1) in Section 2.2, we need to choose one variable to be sensored. Note that in the detonation wave, the pressure, temperature, and density all have a reaction zone (like an "overshoot") and a shock zone. Only the mass fraction $z$ has a clean single shock wave. It can also be seen from the mass fraction equation. Eliminating the density from Eq. (3.4) by using Eq. (3.1), we obtain

$$z_t + uz_x = -K(T)z, \tag{3.9}$$

which is of the scalar type Eq. (2.1). This helps us identify the troubled cell by the variable $z$.

(2) After the troubled cell $I_j$ is identified, we would like to locate the exact shock location $\theta$ by conservation Eq. (2.11) and then extrapolate the variables $\rho z$ and $T$. We observe that the mass fraction $z$ has values 0 or 1 denoted for the burnt gas and unburnt gas, respectively. Thus it is easy to modify the value of $z$ by just taking

$$\tilde{z}_j = \begin{cases} 0, & \theta \geq x_j \\ 1, & \theta < x_j \end{cases} . \tag{3.10}$$

Then it remains to use the temperature $T$ to compute $\theta$ by letting $u = T$ in Eq. (2.11). The new temperature is obtained by the interpolation polynomials in Eq. (2.10). From the numerical experiments, we found that the density $\rho$ is not sensitive to how the source term is computed. Thus for simplicity it remains unchanged.

REMARK 3. *$s = r = 1$ also works well in all the numerical examples for the system case.*

REMARK 4. *First-order extrapolation of temperature can also capture the correct shock speed. However, the order of accuracy will be decreased.*

### 3.3. *Numerical examples of one-dimensional detonation waves*

#### 3.3.1. *Example 1: C-J detonation wave (Arrhenius case)*

The first example is an Arrhenius case. It is from Helzel *et al.* (1999; see also Tosatto & Vigevano 2008). The initial values consist of totally burnt gas on the left-hand side

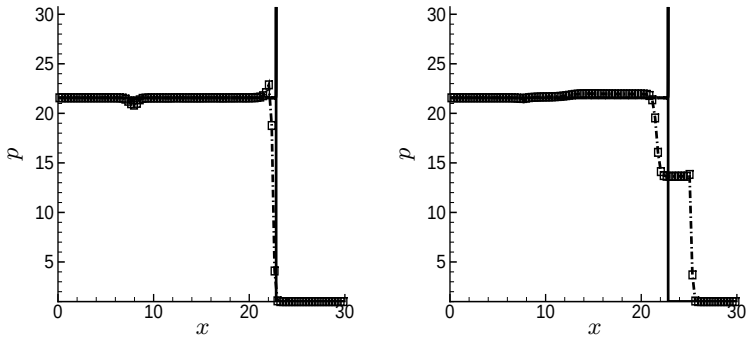


FIGURE 3. Pressure results of the Arrhenius case at $t = 1.8$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 100$, CFL=0.005; right: regular WENO5 with $N = 100$, CFL=0.005.

and totally unburnt gas on the right-hand side. The density, velocity, and pressure of the unburnt gas are given by $\rho_u = 1$, $u_u = 0$ and $p_u = 1$. The heat release $q_0 = 25$ and the ratio of specific heats is set to $\gamma = 1.4$. We consider the ignition temperature $T_{ign} = 25$ and $K_0 = 164180$. We can obtain the C-J initial state for the unburnt gas by, for example, Chorin (1977)

$$p_b = -b + (b^2 - c)^{1/2}, \tag{3.11}$$

$$\rho_b = \frac{\rho_u[p_b(\gamma + 1) - p_u]}{\gamma p_b}, \tag{3.12}$$

$$s_{CJ} = [\rho_u u_u + (\gamma p_b \rho_b)^{1/2}]/\rho_u, \tag{3.13}$$

$$u_b = s_{CJ} - (\gamma p_b/\rho_b)^{1/2}, \tag{3.14}$$

where

$$b = -p_u - \rho_u q_0(\gamma - 1),$$

$$c = p_u^2 + 2(\gamma - 1)p_u \rho_u q_0/(\gamma + 1),$$

and $s_{CJ}$ is the speed of the C-J detonation wave. In this example, $S_{CJ} = 7.1247$.

The computational domain is $[0, 30]$. Initially, the discontinuity is located at $x = 10$. At time $t = 1.8$, the detonation wave has moved to $x = 22.8$. The reference solution is computed by the regular WENO5 scheme with $N = 10000$ ($\Delta x = 0.003$), CFL=0.05.

We compare our proposed WENO5/SR method with the regular WENO5 method on coarse meshes. The pressure, temperature, density and mass fraction results are plotted in Figures 3-6. Only $N = 100$ ($\Delta x = 0.3$) with CFL=0.005 are used in WENO5/SR. It is able to capture the correct propagation speed of the detonation wave. However, the regular WENO5 with the same mesh size produces spurious numerical results. We remark that our method can use fewer points than the previous methods in Helzel *et al.* (1999) and Tosatto & Vigevano (2008) to obtain similar results. The reason may be the high-order accuracy of the spatial scheme in the convection step.

3.3.2. *Example 2: C-J detonation wave (Heaviside case)*

In this example the chemical reaction is modeled by Heaviside form. This example is taken from Colella *et al.* (1986; see also Ben-Artzi 1989 and Bao & Jin 2000).

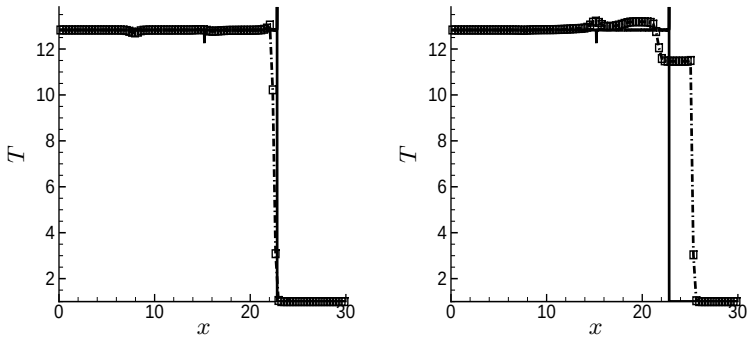


FIGURE 4. Temperature results of the Arrhenius case at $t = 1.8$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 100$, CFL=0.005; right: regular WENO5 with $N = 100$, CFL=0.005.

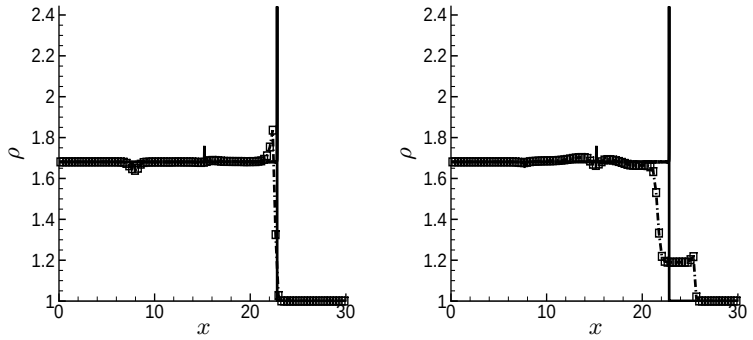


FIGURE 5. Density results of the Arrhenius case at $t = 1.8$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 100$, CFL=0.005; right: regular WENO5 with $N = 100$, CFL=0.005.

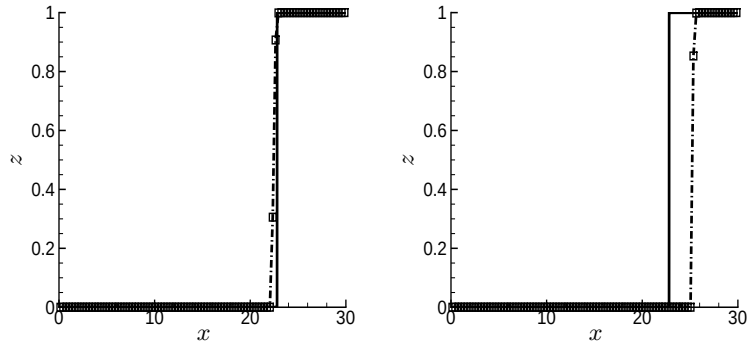


FIGURE 6. Mass fraction results of the Arrhenius case at $t = 1.8$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 100$, CFL=0.005; right: regular WENO5 with $N = 100$, CFL=0.005.

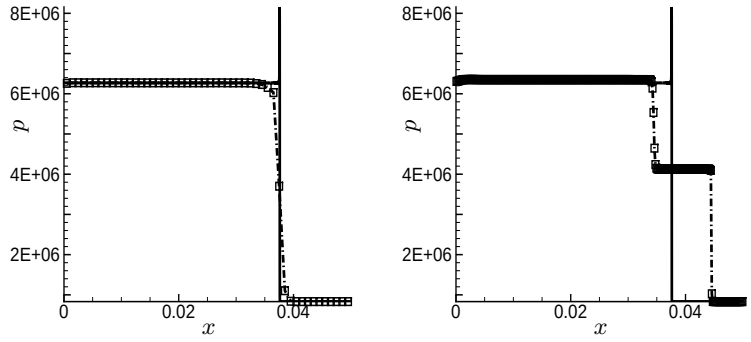


FIGURE 7. Pressure results of Example 2 at $t = 3 \times 10^{-7}$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 50$, CFL=0.005; right: regular WENO5 with $N = 300$, CFL=0.005.

Consider the following parameter values in the CGS units:

$$q_0 = 0.5196 \times 10^{10}, \quad \frac{1}{\varepsilon} = 0.5825 \times 10^{10}, \quad T_{ign} = 0.1155 \times 10^{10}.$$

The computational domain is $[0, 0.05]$. The initial conditions are given by

$$(\rho, u, p, z) = \begin{cases} (\rho_b, u_b, p_b, 0) & x \le 0.005 \\ (1.201 \times 10^{-3}, 0, 8.321 \times 10^5, 1) & x > 0.005 \end{cases}, \tag{3.15}$$

where $\rho_b$, $u_b$ and $p_b$ are computed by Eqs. (3.11)-(3.14). From Eq. (3.13), the speed of the detonation wave in this example is $D_{CJ} = 1.088 \times 10^5$. In this example, the width of the reaction zone is approximately $5 \times 10^{-5}$ (see Ben-Artzi 1989 and Colella *et al.* 1986).

The reference solution is computed by the regular WENO5 scheme with $N = 5000$ points ($\Delta x = 1 \times 10^{-5}$) and CFL=0.05. The solutions are run to time $t = 3 \times 10^{-7}$. The wave moves to $x = 0.03764$. The pressure, temperature, density and mass fraction results are plotted in Figures 7-10. Again we compare the results by WENO5/SR (left subplots) with regular WENO5 (right subplots). We can see WENO5/SR with $N = 50$ is able to capture the correct detonation speed. However, regular WENO5 with $N = 300$ still produces wrong numerical results no matter how small the time step is, which is not shown here.

## 4. Future plans

In this report, we demonstrated that the proposed high-order finite difference schemes with subcell resolution are able to capture the correct discontinuity speed in both one-dimensional scalar and system cases. Future work will extend this approach to higher dimensions with more general chemical reaction models. We will also consider multiple reaction models.

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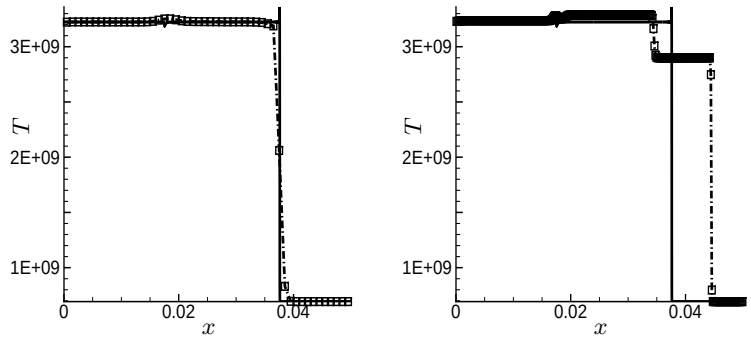


FIGURE 8. Temperature results of Example 2 at $t = 3 \times 10^{-7}$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 50$, CFL=0.005; right: regular WENO5 with $N = 300$, CFL=0.005.

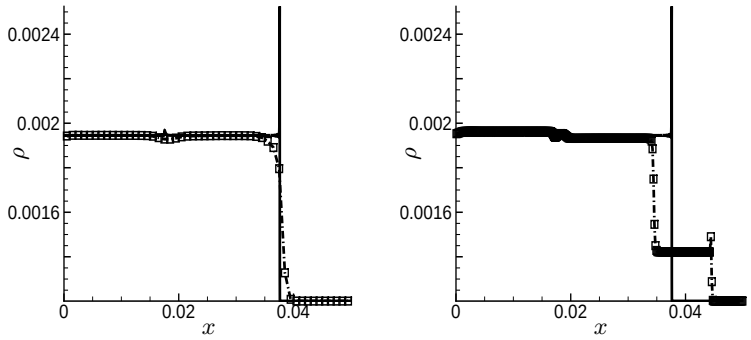


FIGURE 9. Density results of Example 2 at $t = 3 \times 10^{-7}$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 50$, CFL=0.005; right: regular WENO5 with $N = 300$, CFL=0.005.

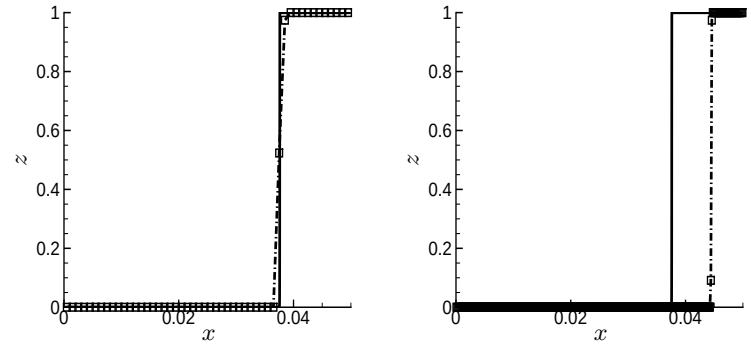


FIGURE 10. Mass fraction results of Example 2 at $t = 3 \times 10^{-7}$. Solid line: the reference solution. Dashed line with symbols: Left: WENO/SR with $N = 50$, CFL=0.005; right: regular WENO5 with $N = 300$, CFL=0.005.

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