Shock Wave Simulations by Finite Difference Schemes

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We consider the one-dimensional motion with strong shock layer for the gas by some finite difference schemes.

$$
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right), \\
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho Eu + pu)}{\partial x} = \frac{\partial}{\partial x}\left(\kappa \frac{\partial \theta}{\partial x} + \mu u \frac{\partial u}{\partial x}\right),
$$

where $\rho$, $u$, $\theta$ are the density, velocity and temperature, the pressure $p$ and internal energy $e$ are functions of the density and temperature, $E = e + u^2/2$, and $\mu$, $\kappa$ are the coefficients of viscosity and heat-conduction. Here we assume for a simplicity the equation of state: $p = R\rho \theta$ and $e = R\theta/\gamma - 1$.

Also we consider the isothermal model: $p = R\rho$ and the barotropic model: $p = R\rho^\gamma$, $\gamma > 1$. The system is the following:

$$
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right),
$$

where $p = R\rho^\gamma$, $\gamma \geq 1$.

The artificial viscosity of Neumann-Richtmyer type may have the following form written as partial differential equations in the Eulerian coordinate.

$$
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \\
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \mu \frac{\partial}{\partial x}\left(|\frac{\partial u}{\partial x}| \frac{\partial u}{\partial x}\right), \\
\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho Eu + pu)}{\partial x} = \mu \frac{\partial}{\partial x}\left(u |\frac{\partial u}{\partial x}| \frac{\partial u}{\partial x}\right).
$$
\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0, \]
\[ \frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \mu \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \right). \]

On the other hand the artificial viscosity of Lax-Friedrichs type may have the following form written as partial differential equations in the Eulerian coordinate:

\[ \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = \epsilon \frac{\partial^2 \rho}{\partial x^2}, \]
\[ \frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = \mu \frac{\partial^2 (\rho u)}{\partial x^2}. \]
\[ \frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho Eu + pu)}{\partial x} = \nu \frac{\partial^2 (\rho E)}{\partial x^2}. \]

Here we transform the above systems of equations to some natural finite difference schemes and compare the shock wave computations by those finite difference schemes.

The following scheme is a simple one for the system with the physical viscosity and heat-conduction.

\[
\rho_j^{k+1} = \rho_j^k - \frac{r}{2} ((\rho u)_j^{k+1} - (\rho u)_{j-1}^k), \\
(\rho u)_j^{k+1} = (\rho u)_j^k - \frac{r}{2} ((\rho u)_{j+1}^k u_{j+1}^k + p_{j+1}^k u_{j+1}^k - (\rho u)_{j-1}^k u_{j-1}^k - p_{j-1}^k u_{j-1}^k) \\
+ s \mu (u_{j+1}^k - 2u_j^k + u_{j-1}^k), \\
(\rho E)_j^{k+1} = (\rho E)_j^k - \frac{r}{2} ((\rho E)_{j+1}^k u_{j+1}^k + p_{j+1}^k u_{j+1}^k - (\rho E)_{j-1}^k u_{j-1}^k - p_{j-1}^k u_{j-1}^k) \\
+ s \{ \kappa (\theta_{j+1}^k - 2\theta_j^k + \theta_{j-1}^k) + \frac{\mu}{2} ((u_{j+1}^k)^2 - 2(u_j^k)^2 + (u_{j-1}^k)^2) \},
\]

where \( r = \Delta t/\Delta x \) and \( s = \Delta t/(\Delta x)^2 \), and the notations \( \rho_j^k = \rho(k \Delta t, j \Delta x) \), \( p_j^k = p(\rho_j^k, \theta_j^k) \) etc. are used.
To see the shock layer profile we introduce the moving frame with the same velocity 
as the shock wave.

\[
\frac{\partial \rho}{\partial t} - \sigma \frac{\partial \rho}{\partial x} + \frac{\partial (\rho u)}{\partial x} = 0 ,
\]

\[
\frac{\partial (\rho u)}{\partial t} - \sigma \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho u^2 + p)}{\partial x} = \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial x} \right) ,
\]

\[
\frac{\partial (\rho E)}{\partial t} - \sigma \frac{\partial (\rho E)}{\partial x} + \frac{\partial (\rho Eu + pu)}{\partial x} = \frac{\partial}{\partial x} \left( \kappa \frac{\partial \theta}{\partial x} + \mu u \frac{\partial u}{\partial x} \right) ,
\]

where \( \sigma \) is the velocity of the shock wave. The shock layer solution becomes stationary.

The Rankine-Hugoniot relation is necessary for the shock layer.

\[
\sigma \left[ \rho_+ - \rho_- \right] = \left[ (\rho u)_+ - (\rho u)_- \right] ,
\]

\[
\sigma \left[ (\rho u)_+ - (\rho u)_- \right] = \left[ (\rho u^2)_+ + p_+ - (\rho u^2)_- - p_- \right] ,
\]

\[
\sigma \left[ (\rho E)_+ - (\rho E)_- \right] = \left[ (\rho Eu + pu)_+ - (\rho Eu + pu)_- \right] .
\]

Let us consider the shock wave with \( \sigma > 0 \). The above finite difference scheme may be changed to the following upwind scheme :

\[
\rho_{j+1}^{k+1} = \rho_j^k + r \sigma (\rho_{j+1}^k - \rho_j^k) - r ((\rho u)_{j+1}^k - (\rho u)_j^k) ,
\]

\[
(\rho u)_{j+1}^{k+1} = (\rho u)_j^k + r \sigma ((\rho u)_{j+1}^k - (\rho u)_j^k)
- r ((\rho u)_{j+1}^k u_{j+1}^k - (\rho u)_j^k u_j^k)
+ s \mu \{ u_{j+1}^k - 2 u_j^k + u_{j-1}^k \} ,
\]

\[
(\rho E)_{j+1}^{k+1} = (\rho E)_j^k + r \sigma ((\rho E)_{j+1}^k - (\rho E)_j^k)
- r ((\rho E)_{j+1}^k + p_{j+1}^k) u_{j+1}^k - ((\rho E)_j^k + p_j^k) u_j^k)
+ s \{ \kappa (\theta_{j+1}^k - 2 \theta_j^k + \theta_{j-1}^k) + \frac{\mu}{2} (u_{j+1}^k)^2 - 2 (u_j^k)^2 + (u_{j-1}^k)^2 \} ,
\]

where \( r = \Delta t/\Delta x \) and \( s = \Delta t/(\Delta x)^2 \).
In the case of barotropic equations the upwind finite difference scheme for the physical viscosity is the following:

\[
\rho_j^{k+1} = \rho_j^k + r \sigma (\rho_{j+1}^k - \rho_j^k) - r ((\rho u_j^k)_{j+1} - (\rho u_j^k)_{j}) , \\
(\rho u_j)^{k+1} = (\rho u_j)^k + r \sigma ((\rho u_j)^k_{j+1} - (\rho u_j)^k_{j}) \\
- r ((\rho u_j)^k_{j+1} u_{j+1}^k - (\rho u_j)^k_j u_j^k) - \frac{r}{2} (p_{j+1}^k - p_{j-1}^k) \\
+ s \mu \{u_{j+1}^k - 2u_j^k + u_{j-1}^k\} .
\]

Here only the pressure term is the centered difference scheme.

We have the following existence theorem of the stationary shock layer for this scheme.

**Theorem**

Let be given the values \( \rho_+ , u_+ , u_- \), which determine the values \( \rho_- \) and \( \sigma \) by Rankine-Hugoniot relation. Let \( v = 1/\rho \). If \( \frac{m}{\Delta x} - \frac{1}{2} p_0 (u_+) > - p_0 (u_-) - m^2 \), where \( m = \sqrt{\frac{p_0 (u_+) - p_0 (u_-)}{u_+ - u_-}} \), then the monotone discrete shock profile exists which connect the values \( (\rho_\pm , u_\pm) \).

**Proof**

We are considering the case : \( \sigma > 0 \). The equations for the stationary shock profile \((\rho_{j+1}^k, u_{j+1}^k) = (\rho_{j}^k, u_{j}^k)\) are the following:

\[
\sigma (\rho_{j+1} - \rho_j) - ((\rho u)_{j+1} - (\rho u)_j) = 0 , \\
\sigma ((\rho u)_{j+1} - (\rho u)_j) - ((\rho u)_{j+1} u_{j+1} - (\rho u)_j u_j) \\
- \frac{1}{2} (p_{j+1} - p_{j-1}) + \frac{\mu}{\Delta x} \{u_{j+1} - 2u_j + u_{j-1}\} = 0 .
\]

Summing up to the left, we have the equations by Rankine-Hugoniot relation.

\[
(\sigma - u_{j+1}) \rho_{j+1} = (\sigma - u_-) \rho_- = m , \\
\frac{\mu}{\Delta x} (u_{j+1} - u_j) = - m (u_{j+1} - u_-) + \frac{1}{2} (p_{j+1} + p_j) - p_- .
\]

If we use \( v_j = 1/\rho_j , u_\pm = 1/\rho_\pm \) and notice

\[
u_{j+1} - u_j = - m (v_{j+1} - v_j) ,
\]
then we have
\[
\frac{\mu m}{\Delta x} (v_{j+1} - v_j) = -m^2 (v_{j+1} - v_-) - (p_{j+1} - p_-) + \frac{1}{2} (p_{j+1} - p_j).
\]
Thus we know
\[
(\frac{\mu m}{\Delta x} - \frac{1}{2} p_v (\tilde{v}))(v_{j+1} - v_j) = -m^2 (v_{j+1} - v_-) - (p_{j+1} - p_-) > 0
\]
by the convexity of \( p(v) \). Therefore if \( v_- < v_{j+1} < v_+ \), then we have \( v_{j+1} > v_j \) and also \( v_j > v_- \) by the assumption.

We show several computations of the isothermal models for a simplicity, which have similar figures to those of the full system. The upper is the velocity profile and the lower is the density. Boundary conditions for computation are Dirichlet for the momentum at both ends and for the density at \( x = x_+ \), and Neumann zero for the density at \( x = 0 \).

The shock profile of upwind scheme with physical viscosity. They are monotone.

\[\text{Figure 1: Upwind scheme with physical viscosity}\]
\[ (\rho_-, u_-) = (5.8284 \cdots, 3.0), (\rho_+, u_+) = (1.0, 1.0), \sigma = 3.4142 \cdots \]
\[ \epsilon = 0.0, \mu = 0.01, \Delta x = 1/512, 0 < x < 2. \]
The semi-upwind difference scheme for the physical viscosity is the following:

\[ \rho_{j}^{k+1} = \rho_{j}^{k} + r \sigma (\rho_{j+1}^{k} - \rho_{j}^{k}) - \frac{r}{2} ((\rho u)_{j+1}^{k} - (\rho u)_{j-1}^{k}), \]
\[ (\rho u)_{j}^{k+1} = (\rho u)_{j}^{k} + r \sigma ((\rho u)_{j+1}^{k} - (\rho u)_{j}^{k}) - \frac{r}{2} ((\rho u)_{j+1}^{k} u_{j+1}^{k} - (\rho u)_{j}^{k} u_{j}^{k}) - r (p_{j+1}^{k} - p_{j-1}^{k}) + s \mu \left\{ u_{j+1}^{k} - 2u_{j}^{k} + u_{j-1}^{k} \right\}. \]

The shock profile of semi-upwind scheme with physical viscosity. They are monotone but less sharp than those of upwind. The computation is more stable.

Figure 2: Semi-upwind with physical viscosity

\[ (\rho_{-}, u_{-}) = (5.8284 \ldots, 3.0), \ (\rho_{+}, u_{+}) = (1.0, 1.0), \ \sigma = 3.4142 \ldots \]
\[ \epsilon = 0.0, \ \mu = 0.01, \ \Delta x = 1/256, \ 0 < x < 2. \]

The upwind finite difference scheme for the artificial viscosity of Neumann-Richtmyer type is the following:

\[ \rho_{j}^{k+1} = \rho_{j}^{k} + r \sigma (\rho_{j+1}^{k} - \rho_{j}^{k}) - r ((\rho u)_{j+1}^{k} - (\rho u)_{j}^{k}), \]
\[ (\rho u)_{j}^{k+1} = (\rho u)_{j}^{k} + r \sigma ((\rho u)_{j+1}^{k} - (\rho u)_{j}^{k}) - r (p_{j+1}^{k} - p_{j-1}^{k}) + s \mu \left\{ u_{j+1}^{k} - u_{j}^{k} |(u_{j+1}^{k} - u_{j}^{k}) - |u_{j}^{k} - u_{j-1}^{k}|(u_{j}^{k} - u_{j-1}^{k}) \right\}. \]
Here we notice about oscillations of Neumann-Richtmyer scheme. In the similar way to the scheme of physical viscosity we have the following equation:

\[
\left( \frac{\mu m^2}{\Delta x} | v_{j+1} - v_j | - \frac{1}{2} p_v(\bar{v}) \right) (v_{j+1} - v_j) = -m^2 (v_{j+1} - v_-) - (p_{j+1} - p_-) > 0
\]

Therefore if \( v_- < v_{j+1} < v_+ \), then we have \( v_{j+1} > v_j \). However when \( v_j \rightarrow v_- \), then the term of left hand side tends to \(-\frac{1}{2} p_v(v_-) (v_{j+1} - v_j)\) but the term of right hand side tends to \((-p_v(v_-) - m^2) (v_{j+1} - v_-)\). In order to have \( v_j > v_- \), \( m^2 > -\frac{1}{2} p_v(v_-) \) is necessary. It is satisfied by the small shocks, but it is violated when the shock becomes strong.

The shock profile of upwind scheme with Neumann-Richtmyer type viscosity. They are oscillating near \((\rho_-, u_-)\) as noticed above.

Figure 3: Upwind with Neumann-Richtmyer viscosity
\((\rho_-, u_-) = (5.8284 \ldots, 3.0), (\rho_+, u_+) = (1.0, 1.0)\), \( \sigma = 3.4142 \ldots \)
\( \epsilon = 0.0, \mu = 0.01, \Delta x = 1/512 \), \( 0 < x < 2 \).
The semi-upwind difference scheme for the artificial viscosity of Neumann-Richtmyer type is the following:

\[
\rho_{j}^{k+1} = \rho_{j}^{k} + r\sigma(\rho_{j+1}^{k} - \rho_{j}^{k}) - \frac{r}{2}((\rho u)_{j+1}^{k} - (\rho u)_{j-1}^{k}),
\]

\[
(\rho u)_{j}^{k+1} = (\rho u)_{j}^{k} + r\sigma((\rho u)_{j+1}^{k} - (\rho u)_{j})
\]

\[\quad - \frac{r}{2}((\rho u)_{j+1}^{k}u_{j+1}^{k} - (\rho u)_{j-1}^{k}u_{j-1}^{k} - (p_{j+1}^{k} - p_{j-1}^{k}))
\]

\[\quad + s\mu \{|u_{j+1}^{k} - u_{j}^{k}|(u_{j+1}^{k} - u_{j}^{k}) - |u_{j}^{k} - u_{j-1}^{k}|(u_{j}^{k} - u_{j-1}^{k})\}.
\]

The shock profile of semi-upwind scheme with Neumann-Richtmyer type viscosity.

They are monotone and a little sharper than those of physical viscosity.

Figure 4: Semi-upwind with Neumann-Richtmyer type viscosity

\((\rho_{-}, u_{-}) = (5.8284\ldots, 3.0), (\rho_{+}, u_{+}) = (1.0, 1.0), \sigma = 3.4142\ldots, \epsilon = 0.0, \mu = 0.01, \Delta x = 1/256, 0 < x < 2.\)
The upwind difference scheme for the artificial viscosity of Lax-Friedrichs type is the following:

\[
\rho^k_j = \rho^k_j + \tau \sigma (\rho^k_{j+1} - \rho^k_j) - \tau ((\rho u)^k_{j+1} - (\rho u)^k_j) + s \epsilon \{-2 \rho^k_j + \rho^k_{j-1}\}
\]

\[
(\rho u)^{k+1}_j = (\rho u)^k_j + \tau \sigma ((\rho u)^{k+1}_j - (\rho u)^k_j)
- \tau ((\rho u)^k_{j+1} u^k_{j+1} - (\rho u)^{k}_j u^k_j) - \frac{\tau}{2} (p^k_{j+1} - p^k_{j-1})
+ s \mu \{(\rho u)^{k+1}_j - 2(\rho u)^k_j + (\rho u)^{k}_j\}.
\]

The shock profile of Upwind scheme with Lax-Friedrichs type viscosity.

They are monotone.

Figure 5: Upwind of Lax-Friedrichs type

\((\rho_-, u_-) = (5.8284 \cdots, 3.0), (\rho_+, u_+) = (1.0, 1.0), \sigma = 3.4142 \cdots, \epsilon = 0.005, \mu = 0.005, \Delta x = 1/256, 0 < x < 2\).
The semi-upwind difference scheme for the artificial viscosity of Lax-Friedrichs type is the following:

\[
\rho_{j}^{k+1} = \rho_{j}^{k} + \sigma \left( \rho_{j+1}^{k} - \rho_{j}^{k} \right) - \frac{r}{2} \left( (\rho u)_{j+1}^{k} - (\rho u)_{j}^{k} \right) + s \epsilon \left\{ \rho_{j+1}^{k} - 2 \rho_{j}^{k} + \rho_{j-1}^{k} \right\} (\rho u)_{j}^{k+1} = (\rho u)_{j}^{k} + \sigma \left( \rho_{j+1}^{k} - \rho_{j}^{k} \right) - \frac{r}{2} \left\{ (\rho u)_{j+1}^{k} u_{j+1}^{k} - (\rho u)_{j-1}^{k} u_{j-1}^{k} - (p_{j+1}^{k} - p_{j-1}^{k}) \right\} + s \mu \left\{ (\rho u)_{j+1}^{k} - 2 (\rho u)_{j}^{k} + (\rho u)_{j-1}^{k} \right\} .
\]

The shock profile of semi-upwind scheme with an artificial viscosity of Lax-Friedrichs type. They are not monotone.

\[
\rho_{-}, u_{-} = (5.8284 \cdots, 3.0) , \ (\rho_{+}, u_{+}) = (1.0, 1.0) , \ \sigma = 3.4142 \cdots \\
\epsilon = 0.1 , \ \mu = 0.0 , \ \Delta x = 1/256 , \ 0 < x < 2 .
\]
The shock profile of semi-upwind scheme with an artificial viscosity.
They are highly oscillatory. The difference from the previous profile is the $x-$ interval of computations.

Figure 7: Semi-upwind of an artificial viscosity
$(\rho_-, u_-) = (5.8284 \cdots, 3.0)$, $(\rho_+, u_+) = (1.0, 1.0)$, $\sigma = 3.4142 \cdots$
$\epsilon = 0.1$, $\mu = 0.0$, $\Delta x = 1/256$, $0 < x < 4$
Snap-shot at $t = 64.0, 64.25, 64.5, 64.75, 65.0$.

Figure 8 is the shock profile of semi-upwind scheme with another artificial viscosity of Lax-Friedrichs type. They are monotone but less sharp. When the $x-$ interval of computation is enlarged or $\mu$ is getting bigger, the scheme becomes unstable for time evolution.

As a whole the finite difference scheme with the physical viscosity works better.
Figure 8: Semi-upwind of another artificial viscosity
\[(\rho_-, u_-) = (5.8284\cdots, 3.0) , \ (\rho_+, u_+) = (1.0, 1.0) , \ \sigma = 3.4142\cdots \]
\[\epsilon = 0.0 , \ \mu = 0.01 , \ \Delta x = 1/256 , \ 0 < x < 2.\]

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