Innovative numerical methods for evolutionary partial differential equations and applications

Numerical validation of homogeneous multi-fluid models

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Outline

1. Problem setup
2. Detailed numerical solution
3. Numerical tests
4. Multi-fluid models
5. Numerical comparison
Problem setup

Figure: Homogeneous limit of a multi-fluid system.
Mass Lagrangian coordinates

We shall make use of the mass Lagrangian coordinates

$$\xi = \int_0^x \rho(z, t) \, dz = \int_0^X \rho_0(z) \, dz. \tag{1.1}$$

where $x$ is the Eulerian coordinate, $X$ is the initial position of fluid particles and $\rho_0(X)$ is the initial density. The Lagrangian coordinates $\xi$ corresponding to the position $x$ is the mass from the origin of the tube $x_0 = 0$, to $x$.

**Figure:** Describing the mass defined by Lagrangian coordinates
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Let us consider the Euler equations in Lagrangian coordinates

\[
\frac{DU}{Dt} + \frac{\partial f(U)}{\partial \xi} = 0,
\]  

(2.1)
Governing equations

Let us consider the Euler equations in Lagrangian coordinates

\[
\frac{DU}{Dt} + \frac{\partial f(U)}{\partial \xi} = 0, \tag{2.1}
\]

where

\[
U = \begin{pmatrix} V \\ u \\ E \end{pmatrix}, \quad f(U) = \begin{pmatrix} -u \\ \rho \\ up \end{pmatrix}. \tag{2.2}
\]

\(V = 1/\rho\) denotes the specific volume, \(E = \frac{1}{2}u^2 + e\), where \(e = e(V, p)\) denotes the specific internal energy.

The time derivative is Lagrangian derivative has the form

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}. \tag{2.3}
\]
The Jacobian matrix of the flux $df(U)/dU$ has the eigenvalues

$$\lambda_1 = -C, \quad \lambda_2 = 0, \quad \lambda_3 = C,$$

(2.4)
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\[
\lambda_1 = -C, \quad \lambda_2 = 0, \quad \lambda_3 = C, \quad (2.4)
\]

where \( C \) denotes the Lagrangian sound velocity.

For ideal gas

\[
e = \frac{pV}{\gamma - 1}, \quad C^2 = \frac{\gamma p}{V}. \quad (2.5)
\]

For stiff fluid

\[
e = \frac{(p + \gamma p_\infty)V}{\gamma - 1}, \quad C^2 = \frac{\gamma(p + p_\infty)}{V} \quad (2.6)
\]
Finite volume method

We divide the total mass into intervals of the length
\[ \Delta \xi_i = \xi_{i+1/2} - \xi_{i-1/2}. \]

Figure: Setting up for one pair of layer
Finite volume method

- Integrating (2.1) over \([\xi_{i-1/2}, \xi_{i+1/2}]\) gives

\[
\frac{d \langle U \rangle_i}{dt} + \frac{f(U(\xi_{i+1/2}, t)) - f(U(\xi_{i-1/2}, t))}{\Delta \xi_i} = 0, \quad (2.7)
\]

where \(\langle U \rangle_i = \frac{1}{\Delta \xi_i} \int_{\xi_{i-1/2}}^{\xi_{i+1/2}} U(\xi, t) d\xi\) and \(f(U(\xi_{i+1/2}, t))\) is the flux evaluated at \(\xi_{i+1/2}\.\)
Finite volume method

- Integrating (2.1) over \([\xi_{i-1/2}, \xi_{i+1/2}]\) gives

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where \(< U >_i = \frac{1}{\Delta \xi_i} \int_{\xi_{i-1/2}}^{\xi_{i+1/2}} U(\xi, t) d\xi\) and \(f(U(\xi_{i+1/2}, t))\) is the flux evaluated at \(\xi_{i+1/2}\).

We use \(U_i \approx < U >_i\) and replace \(f(U(\xi_{i+1/2}, t))\) by the approximating numerical flux \(F_{i+1/2}\).

- Second order (in space):

\[
F_{i+1/2} = F(U_{i+1/2}^-, U_{i+1/2}^+). \quad (2.8)
\]
\( U_{i+1/2}^- \) and \( U_{i+1/2}^+ \) can be reconstructed by using second order method with the minmod limiter:

\[
U_{i+1/2}^- = U_i + U_i' \frac{\Delta \xi_i}{2}, \quad U_{i+1/2}^+ = U_{i+1} - U_{i+1}' \frac{\Delta \xi_{i+1}}{2}, \quad (2.9)
\]
\( U^{-}_{i+1/2} \) and \( U^{+}_{i+1/2} \) can be reconstructed by using second order method with the minmod limiter:

\[
U^{-}_{i+1/2} = U_i + U'_i \frac{\Delta \xi_i}{2}, \quad U^{+}_{i+1/2} = U_{i+1} - U'_{i+1} \frac{\Delta \xi_{i+1}}{2}, \quad (2.9)
\]

Minmod slope for 3 parameters

\[
U'_i = 2\text{MM}\left( \frac{\theta(U^n_{i+1} - U^n_i)}{\Delta \xi_i + \Delta \xi_{i+1}}, \frac{U^n_{i+1} - U^n_{i-1}}{\Delta \xi_{i-1} + 2\Delta \xi_i + \Delta \xi_{i+1}}, \frac{\theta(U^n_i - U^n_{i-1})}{\Delta \xi_{i-1} + \Delta \xi_{i+1}} \right)
\]

where \( \text{MM} \) is the minmod limiter has the form

\[
\text{minmod3}(a, b, c) = \\
\begin{cases} 
  \min(|a|, |b|, |c|)\text{sign}(a) & \text{if } a, b, c \text{ have the same sign} \\
  0 & \text{if } a, b, c \text{ do not have the same sign}
\end{cases}
\]
High order (in time) numerical scheme

The equation (2.7) can be written as follows

\[
\frac{dU_i}{dt} = - \frac{F_{i+1/2} - F_{i-1/2}}{\Delta \xi} =: \mathcal{F}_i.
\]  

(2.10)
Heun’s method

We obtain the system of equations as follows

$$\frac{dU}{dt} = F$$  \hspace{1cm} (2.11)

where

$$U = \begin{pmatrix} U_1 \\ \vdots \\ U_N \end{pmatrix} \quad \text{and} \quad F = \begin{pmatrix} F_1 \\ \vdots \\ F_N \end{pmatrix}$$  \hspace{1cm} (2.12)

We will use Heun’s method which is second order accurate in time and \textit{strong stability-preserving}.
In order to generate a numerical solution, we follow 4 steps as follows

- **Step 1** $K_1 = \mathcal{F}(U^n)$,
- **Step 2** $\tilde{U} = U^n + \Delta tK_1$,
- **Step 3** $K_2 = \mathcal{F}(\tilde{U})$,
- **Step 4** $U^{n+1} = U^n + \Delta t(K_1 + K_2)/2$. 
Roe Flux based on the composition of flux’s jump

\[
F_{\text{newROE}}(U_l, U_r) = \frac{1}{2} \left( F(U_l) + F(U_r) \right) - \frac{1}{2} \sum_{j=1}^{3} \text{sign}(\lambda_j^{\text{ROE}}) \alpha_j r_j,
\]

(2.13)

where \( \alpha_j \) is the coefficient defined by solving the system

\[
F(U_r) - F(U_l) = \frac{1}{2} \sum_{j=1}^{3} \text{sign}(\lambda_j^{\text{ROE}}) \alpha_j r_j.
\]

Roe Flux based on the composition of flux’s jump

\[
F_{\text{newROE}}(U_l, U_r) = \frac{1}{2} \left( F(U_l) + F(U_r) \right) - \frac{1}{2} \sum_{j=1}^{3} \text{sign}(\lambda_{j}^{ROE}) \alpha_j r_j,
\]

(2.13)

where \( \alpha_j \) is the coefficient defined by solving the system

\[
F(U_r) - F(U_l) = \sum_{j=1}^{3} \alpha_j r_j.
\]

(2.14)

This is the numerical flux obtained following Roe’s idea by decomposing the flux instead of the conservative variables.

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Multi-layer tube

We consider a tube filled by $n_p$ pairs of layers, each pair consists of 2 layers of 2 different fluids. The initial condition for the velocity $u$, pressure denoted by $p$ and the initial density satisfies

\[
\rho = \bar{\rho} \left( \frac{p + p_{\infty}}{\bar{p} + p_{\infty}} \right)^{\frac{1}{\gamma}}, \quad \bar{\rho} \text{ is the middle point of the domain with length of 10, } \bar{p} = p_{10} = p_{20} = 10 \text{ and } \bar{\rho} \text{ is } \rho_{10} = 20 \text{ or } \rho_{20} = 10, \quad p_{\infty} \text{ is stiffness parameter, } p_{\infty1} = 100, \quad p_{\infty2} = 0, \quad \gamma_1 = 4.4 \text{ and } \gamma_2 = 1.4 \text{ corresponding to the position in the tube.} 
\]
Wave interaction among small number of layers

We consider a tube with \( n_p = 5 \) and the following initial condition

\[
\begin{align*}
\rho_L &= 40, \ u_L = 0.9452, & \text{if } 0 \leq x \leq 1 \\
\rho_R &= 10, \ u_R = 0, & \text{if } 1 < x \leq 10,
\end{align*}
\]

(3.1)

and the initial density satisfies

\[
\rho = \bar{\rho} \left( \frac{p + p_\infty}{\bar{p} + p_\infty} \right)^{\frac{1}{\gamma}}.
\]
Wave interaction among small number of layers

Figure: Velocity profiles of shock propagating in the tube from the initial time up to final time $T_{\text{final}} = 3$. Result is plotted in Eulerian coordinates.
Wave interaction among small number of layers

Figure: Velocity profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Lagrangian coordinates.
Wave interaction among small number of layers

**Figure**: Pressure profiles of shock propagating in the tube from the initial time up to final time $T_{\text{final}} = 3$. Result is plotted in Eulerian coordinates.
Wave interaction among small number of layers

Figure: Pressure profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Lagrangian coordinates.
Wave interaction among small number of layers

Figure: Density profiles of shock propagating in the tube from the initial time up to final time $T_{\text{final}} = 3$. Result is plotted in Eulerian coordinates.
Wave interaction among small number of layers

Figure: Density profiles of shock propagating in the tube from the initial time up to final time $T_{\text{final}} = 3$. Result is plotted in Lagrangian coordinates.
We consider a initial condition with velocity is zero, a smooth pressure profile of the form

\[
\begin{aligned}
\rho &= 10 + M \left(1 + \cos \left( \frac{2\pi}{L} (x - \bar{x}) \right) \right), \quad \text{if } |x - \bar{x}| < L/2 \\
\rho &= 10, \quad \text{if } |x - \bar{x}| \geq L/2
\end{aligned}
\]  

(3.2)

and the initial density satisfies \( \rho = \bar{\rho} \left( \frac{p + p_{\infty}}{\bar{\rho} + p_{\infty}} \right)^{\frac{1}{\gamma}}. \)
Initial condition with $M = 5, L = 5$. 

Figure: Initial condition.
Result with $M = 5$, $L = 5$. Numerical flux: Roe Flux based on the composition of flux’s jump

**Figure:** Result with 20 pairs of layers, 50 points for each pair.
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Isentropic homogeneous model (2x2 model)

Considering isentropic Euler equations corresponding to the conservation of mass and momentum in Lagrangian coordinates

\[
\begin{align*}
V_t - u\xi &= 0 \\
u_t + p\xi &= 0,
\end{align*}
\] (4.1)

Relation \( V = V(p) \) for the mixture

\[
V = Y_1 V_{10} \left( \frac{p + p_{\infty,1}}{p_{10} + p_{\infty,1}} \right)^{-\frac{1}{\gamma_1}} + Y_2 V_{20} \left( \frac{p + p_{\infty,2}}{p_{20} + p_{\infty,2}} \right)^{-\frac{1}{\gamma_2}},
\] (4.2)

where \( Y_1 \) and \( Y_2 \) are the mass fraction of each phase.
3x3 system with turbulent energy

The system in Lagrangian form

\[
\begin{align*}
V_t - u_\xi &= 0, \\
u_t + \tilde{p}_\xi &= 0, \\
\epsilon_t + (u\tilde{p})_\xi &= 0,
\end{align*}
\]

where \( V = \frac{1}{\rho} \), \( \epsilon = e + \frac{u^2}{2} + Vk \), \( \tilde{p} = p + 2k \) and \( e = Y_1 e_1 + Y_2 e_2 \) is the specific internal energy of the mixture,

\[
e_1 = \frac{p + \gamma_1 p_\infty 1L}{\gamma_1 - 1} V_1, \quad e_2 = \frac{p + \gamma_2 p_\infty 2}{\gamma_2 - 1} V_2.
\]

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Data for two cases

- Case 1: $\rho_{10}/\rho_{20} = 2$
- Case 2: $\rho_{10}/\rho_{20} = 10$

<table>
<thead>
<tr>
<th>Reference data</th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{10}$</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$\rho_{10}$</td>
<td>20</td>
<td>100</td>
</tr>
<tr>
<td>$p_{\infty,1}$</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>4.4</td>
<td>4.4</td>
</tr>
<tr>
<td>$p_{20}$</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$\rho_{20}$</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>$p_{\infty,1}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>1.4</td>
<td>1.4</td>
</tr>
</tbody>
</table>

**Table:** Reference states of the multilayer tube
Figure: Comparison between numerical solution of multi-fluid and homogeneous models before shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.3$. 
Figure: Comparison between numerical solution of multi-fluid and homogeneous models before shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 2.5$. 
Numerical results after shock formation

Figure: Comparison between numerical solution of multi-fluid and homogeneous models after shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.3$ (strong shock).
Using Gaussian blurring to smooth out numerical solutions

\[ U_i = \frac{1}{2}(U_{i-1} + U_{i+1}). \]  \hspace{1cm} (5.1)
Numerical results after shock formation

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models for the case of density ratio $\rho_{10}/\rho_{20} = 2$. 
Numerical results after shock formation

**Figure:** Comparison between numerical solution of multi-fluid and homogeneous models after shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 2.5$ (strong shock).
Numerical results after shock formation

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models for the case density ratio $\rho_{10}/\rho_{20} = 10$. 
We consider the test with the following initial condition for the pressure

$$p = \begin{cases} 50, & \text{if } x \leq 5 \\ 10, & \text{if } x > 5 \end{cases} \quad (5.2)$$

where $x \in [0, 10]$. The initial velocity is zero everywhere and the initial density satisfies $\rho = \bar{\rho} \left( \frac{\rho + \rho_\infty}{\bar{\rho} + \rho_\infty} \right)^{\frac{1}{\gamma}}$. For the $3 \times 3$ model $k$ is also zero.
Figure: Comparison between detailed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.5$. 

**Problem setup**

**Detailed numerical solution**

**Numerical tests**

**Multi-fluid models**

**Numerical comparison**

Riemann problem for multi-fluid
Riemann problem for multi-fluid

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.5$. 
Riemann problem for multi-fluid

Figure: Comparison between detailed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 3$. 
Riemann problem for multi-fluid

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 3$. 
The initial condition of the travelling shock for $2 \times 2$ system is

$$
\begin{cases}
    p_L = 40, \ u_L = 0.9452, & \text{if } 0 \leq x \leq 1 \\
    p_R = 10, \ u_R = 0, & \text{if } 1 < x \leq 10,
\end{cases}
$$

and the initial density satisfies

$$
\rho = \bar{\rho} \left( \frac{p + p_\infty}{\bar{p} + p_\infty} \right)^{\frac{1}{\gamma}}.
$$

At $x = 10$ we impose wall conditions: $u = 0$, $\partial p / \partial \xi = 0$. 

Travelling shock - moderate density ratio
Numerical results before hitting the wall

**Figure:** Comparison between smoothed detailed numerical solution, 2 × 2 system, 3 × 3 system before hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 2.5$. 
Numerical results after hitting the wall

Figure: Comparison between smoothed detailed numerical solution, $2 \times 2$ system, $3 \times 3$ system after hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 5$. 
The initial condition of the Riemann problem is

\[
\begin{cases}
  p_L = 40, \quad u_L = 0.5286, & \text{if } x \leq 1 \\
  p_R = 10, \quad u_R = 0, & \text{if } x > 1,
\end{cases}
\]  

(5.4)

where \( x \in [0, 10] \).

The initial density satisfies

\[ \rho = \rho_0 \left( \frac{p + p_\infty}{\rho_0 + p_\infty} \right)^{\frac{1}{\gamma}}. \]
Numerical results before hitting the wall

Figure: Comparison between smoothed detailed numerical solution, 2 × 2 system, 3 × 3 system before hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 5$. 
Numerical results after hitting the wall

Figure: Comparison between smoothed detailed numerical solution, 2 × 2 system, 3 × 3 system after hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 9.5$. 
Comparison of the computation time

<table>
<thead>
<tr>
<th>Detailed computation</th>
<th>$2 \times 2$ system</th>
<th>$3 \times 3$ system</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.8</td>
<td>42.8</td>
<td>50.1</td>
</tr>
</tbody>
</table>

**Table:** Comparison of the computation time (seconds) among the computations of the detailed numerical solution and the two homogeneous models

**Conclusion:** It is much more expensive to perform the detailed numerical simulation than to numerically solve the homogeneous models.
Discussion and conclusion

- For smooth solutions (in pressure and velocity) the two models are both in very good agreement with the detailed numerical solution of multilayer Euler equations.
- When a shock develops, the multilayer solution becomes highly oscillatory and transforms to a dispersive shock for large amplitude shocks.
  - For moderate density ratio, the $2 \times 2$ model gives a better prediction of the shock position.
  - For large density ratio, the turbulent $3 \times 3$ model is in better agreement with a smoothed out version of the detailed numerical compared with the simple $2 \times 2$ model.
- Open problem: construction of non isentropic homogenized models.
https://doi.org/10.1016/j.amc.2022.127693
Thank you for your attention!