Innovative numerical methods for evolutionary partial differential equations and applications

Numerical validation of homogeneous multi-fluid models

Speaker: Dr. Phan Thi My Duyen
Joint work with: Prof. Giovanni Russo
and Prof. Sergey Gavrilyuk

University of Catania, Italy

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Outline

Problem setup

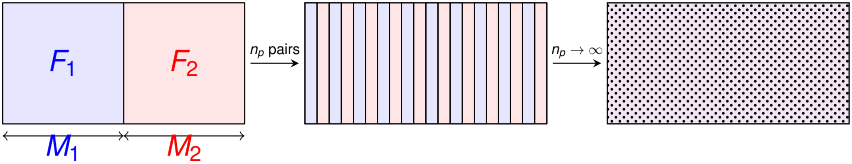

Figure: Homogeneous limit of a multi-fluid system.

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 ξ corresponding to the position x is the mass from the origin of the tube $x_0 = 0$, to x.

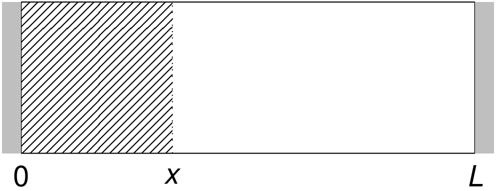

Figure: Describing the mass defined by Lagrangian coordinates

Outline

Governing equations

Let us consider the Euler equations in Lagrangian coordinates

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

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where

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

$V = 1/\rho$ 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

$$\lambda_1 = -C, \quad \lambda_2 = 0, \quad \lambda_3 = C, \tag{2.4}$$

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where C denotes the Lagrangian sound velocity.

- For ideal gas

$$e = \frac{pV}{\gamma - 1}, \quad C^2 = \frac{\gamma p}{V}. \tag{2.5}$$

- For stiff fluid

$$e = \frac{(p + \gamma p_\infty)V}{\gamma - 1}, \quad C^2 = \frac{\gamma(p + p_\infty)}{V} \tag{2.6}$$

Finite volume method

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

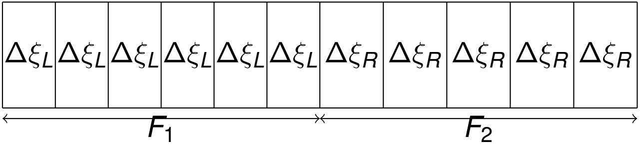

Figure: Setting up for one pair of layer

Finite volume method

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

$$\frac{d < U >_i}{dt} + \frac{f(U(\xi_{i+1/2}, t)) - f(U(\xi_{i-1/2}, t))}{\Delta \xi_i} = 0, \qquad (2.7)$$

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

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  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):

$$F_{i+1/2} = F(U^-_{i+1/2}, U^+_{i+1/2}). \qquad (2.8)$$

- $U^-_{i+1/2}$ and $U^+_{i+1/2}$ can be reconstructed by using second order method with the minmod limiter:

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

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- Minmod slope for 3 parameters

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

where *MM* is the minmod limiter has the form

$$\mathrm{minmod3}(a, b, c) = \begin{cases} \min(|a|, |b|, |c|)\mathrm{sign}(a) & \text{if } a, b, c \text{ have the same sign} \\ 0 & \text{if } a, b, c \text{ do not have the same sign} \end{cases}$$

High order (in time) numerical scheme

The equation (2.7) can be written as follows

$$\frac{dU_i}{dt} = -\frac{F_{i+1/2} - F_{i-1/2}}{\Delta\xi} =: \mathscr{F}_i. \tag{2.10}$$

Heun's method

We obtain the system of equations as follows

$$\frac{dU}{dt} = \mathscr{F} \tag{2.11}$$

where

$$U = \begin{pmatrix} U_1 \\ \vdots \\ U_N \end{pmatrix} \quad \text{and} \quad \mathscr{F} = \begin{pmatrix} \mathscr{F}_1 \\ \vdots \\ \mathscr{F}_N \end{pmatrix} \tag{2.12}$$

We will use Heun's method which is second order accurate in time and *strong stability-preserving*.

Heun's method

In order to generate a numerical solution, we follow 4 steps as follows

- Step 1 $K_1 = \mathscr{F}(U^n)$,
- Step 2 $\tilde{U} = U^n + \Delta t K_1$,
- Step 3 $K_2 = \mathscr{F}(\tilde{U})$,
- Step 4 $U^{n+1} = U^n + \Delta t(K_1 + K_2)/2$.

Roe Flux based on the composition of flux's jump

$$F_{newROE}(U_l, U_r) = \frac{1}{2}\Big(F(U_l) + F(U_r)\Big) - \frac{1}{2}\sum_{j=1}^{3} sign(\lambda_j^{ROE})\alpha_j r_j, \tag{2.13}$$

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where α_j is the coefficient defined by solving the system

$$F(U_r) - F(U_l) = \sum_{j=1}^{3} \alpha_j r_j. \tag{2.14}$$

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

C. D. Munz. "On Godunov-Type Schemes for Lagrangian Gas Dynamics". In: SIAM Journal on Numerical Analysis 31.1 (Feb. 1994), pp. 17-42.

Outline

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 $\rho = \bar{\rho}\left(\frac{p+p_\infty}{\bar{p}+p_\infty}\right)^{\frac{1}{\gamma}}$, $\bar{x}$ is the middle point of the domain with length of 10, $\bar{p} = p_{10} = p_{20} = 10$ and $\bar{\rho}$ is $\rho_{10} = 20$ or $\rho_{20} = 10$, p_∞ is stiffness parameter, $p_{\infty 1} = 100$, $p_{\infty 2} = 0$, $\gamma_1 = 4.4$ and $\gamma_2 = 1.4$ 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

$$\begin{cases} p_L = 40, u_L = 0.9452, & \text{if } 0 \leq x \leq 1 \\ p_R = 10, u_R = 0, & \text{if } 1 < x \leq 10, \end{cases} \tag{3.1}$$

and the initial density satisfies $\rho = \bar{\rho}\Big(\dfrac{p + p_\infty}{\bar{p} + p_\infty}\Big)^{\frac{1}{\gamma}}$.

Wave interaction among small number of layers

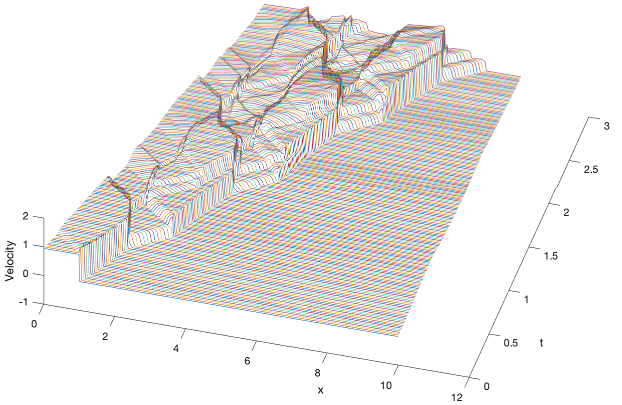

Figure: Velocity profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Eulerian coordinates

Wave interaction among small number of layers

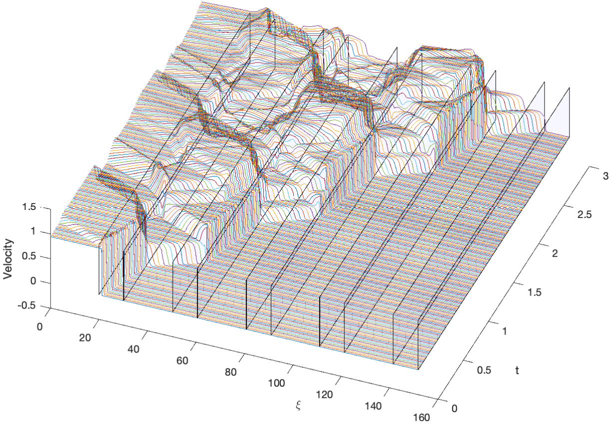

Figure: Velocity profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Lagrangian coordinates

Wave interaction among small number of layers

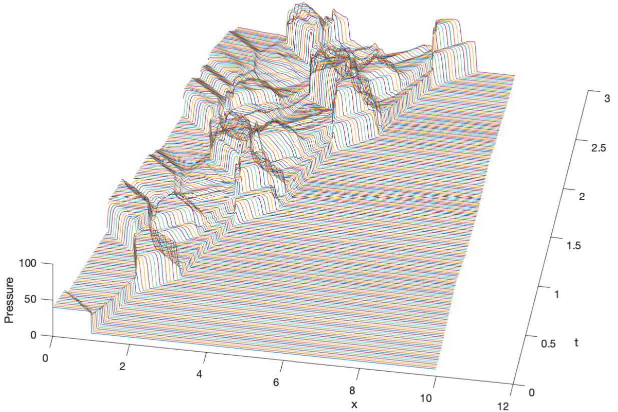

Figure: Pressure profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Eulerian coordinates

Wave interaction among small number of layers

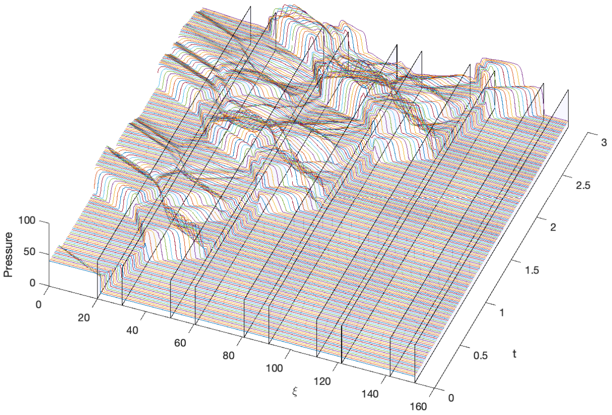

Figure: Pressure profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Lagrangian coordinates

Wave interaction among small number of layers

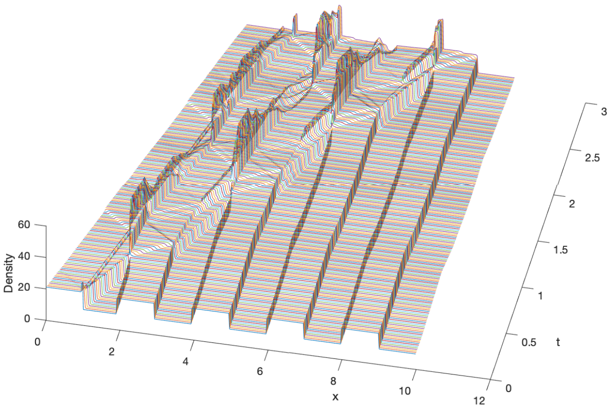

Figure: Density profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Eulerian coordinates

Wave interaction among small number of layers

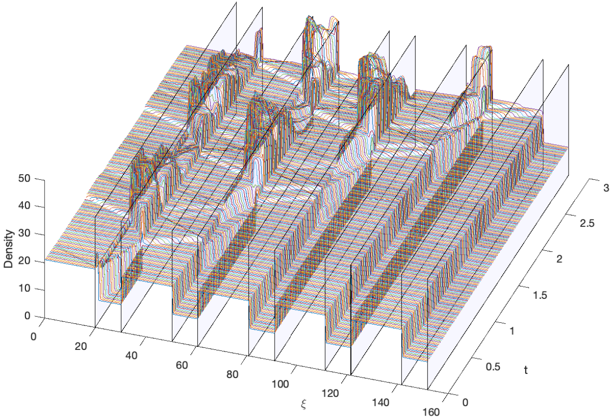

Figure: Density profiles of shock propagating in the tube from the initial time up to final time $T_{final} = 3$. Result is plotted in Lagrangian coordinates

We consider a initial condition with velocity is zero, a smooth pressure profile of the form

$$\begin{cases} p = 10 + M\left(1 + \cos\left(\frac{2\pi(x-\bar{x})}{L}\right)\right), & \text{if } |x - \bar{x}| < L/2 \\ p = 10, \quad \text{if } |x - \bar{x}| \geq L/2 \end{cases} \tag{3.2}$$

and the initial density satisfies $\rho = \bar{\rho}\left(\dfrac{p + p_\infty}{\bar{p} + p_\infty}\right)^{\frac{1}{\gamma}}$.

Initial condition with M = 5, L = 5.

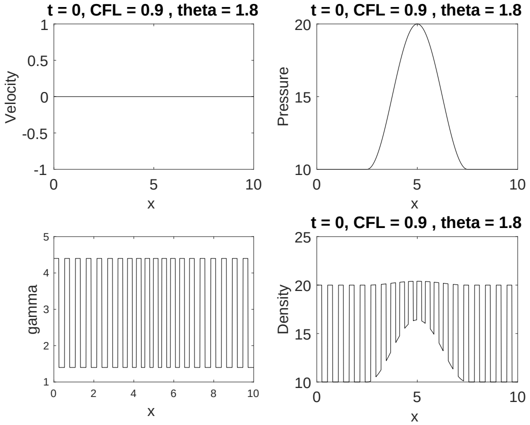

Figure: Initial condition.

Result with M = 5, L = 5. Numerical flux: Roe Flux based on the composition of flux's jump

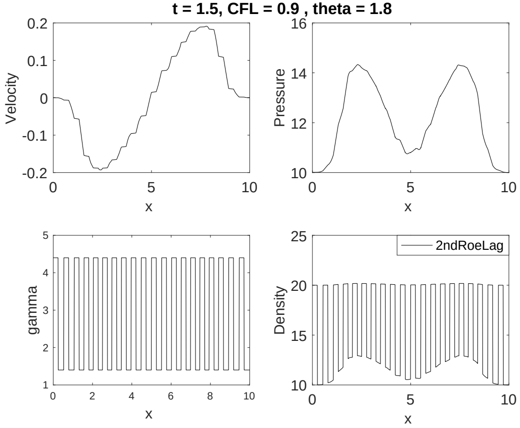

Figure: Result with 20 pairs of layers, 50 points for each pair.

Outline

Isentropic homogeneous model (2x2 model)

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

$$\begin{cases} V_t - u_\xi = 0 \\ u_t + p_\xi = 0, \end{cases} \tag{4.1}$$

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

$$V = Y_1 V_{10}\Big(\frac{p + p_{\infty,1}}{p_{10} + p_{\infty,1}}\Big)^{-\frac{1}{\gamma_1}} + Y_2 V_{20}\Big(\frac{p + p_{\infty,2}}{p_{20} + p_{\infty,2}}\Big)^{-\frac{1}{\gamma_2}}, \tag{4.2}$$

where Y_1 and Y_2 are the mass fraction of each phase.

3x3 system with turbulent energy

The system in Lagrangian form

$$\begin{cases} V_t - u_\xi = 0, \\ u_t + \tilde{p}_\xi = 0, \\ \epsilon_t + (u\tilde{p})_\xi = 0, \end{cases} \tag{4.3}$$

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,

$$e_1 = \frac{p + \gamma_1 p_{\infty 1L}}{\gamma_1 - 1} V_1, \quad e_2 = \frac{p + \gamma_2 p_{\infty 2}}{\gamma_2 - 1} V_2. \tag{4.4}$$

S. L. Gavrilyuk and R. Saurel. "Rankine-Hugoniot relations for shocks in heterogeneous mixtures". In: Journal of Fluid Mechanics 575 (Mar. 2007), pp. 495-507.

Outline

Data for two cases

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

Reference data	Case 1	Case 2
p_{10}	10	10
ρ_{10}	20	100
$p_{\infty,1}$	100	100
γ_1	4.4	4.4
p_{20}	10	10
ρ_{20}	10	10
$p_{\infty,1}$	0	0
γ_2	1.4	1.4

Table: Reference states of the multilayer tube

Numerical results before shock formation

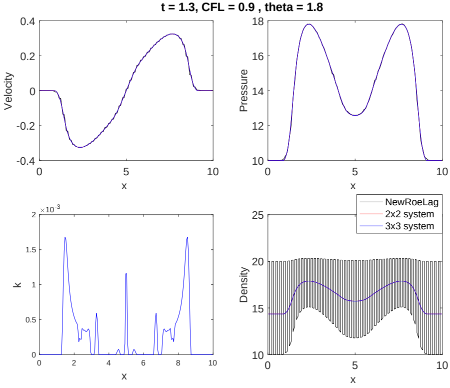

Figure: Comparison between numerical solution of multi-fluid and homogeneous models before shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.3$.

Numerical results before shock formation

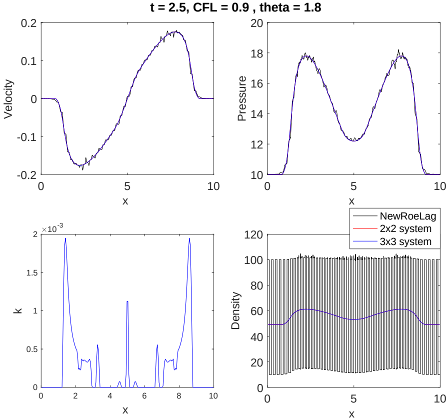

Figure: Comparison between numerical solution of multi-fluid and homogeneous models before shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 2.5$.

Numerical results after shock formation

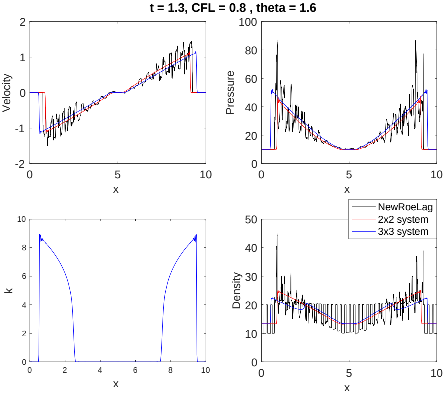

Figure: Comparison between numerical solution of multi-fluid and homogeneous models after shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.3$ (strong shock).

Using Gaussian blurring to smooth out numerical solutions

$$U_i = \frac{1}{2}(U_{i-1} + U_{i+1}). \tag{5.1}$$

Numerical results after shock formation

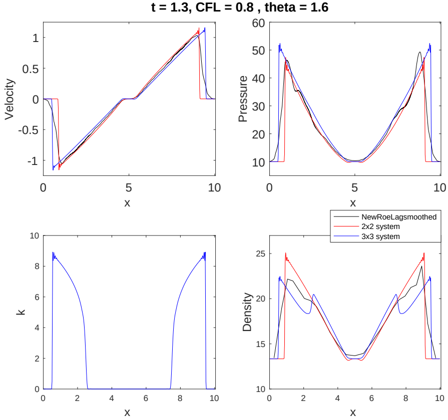

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models for the case of density ratio $\rho_{10}/\rho_{20} = 2$.

Numerical results after shock formation

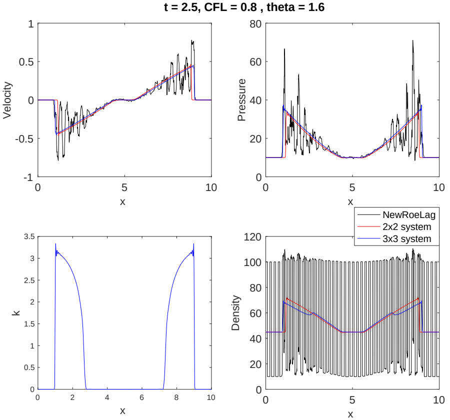

Figure: Comparison between numerical solution of multi-fluid and homogeneous models after shock formation for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 2.5$ (strong shock).

Numerical results after shock formation

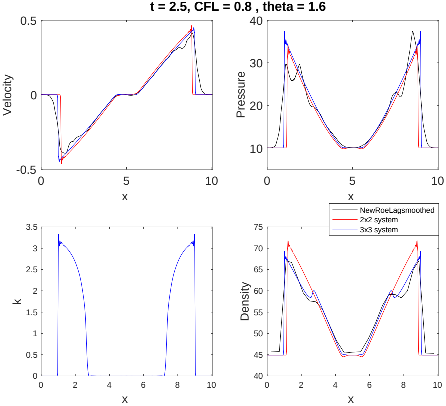

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models for the case density ratio $\rho_{10}/\rho_{20} = 10$.

Riemann problem for multi-fluid

We consider the test with the following initial condition for the pressure

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

where $x \in [0, 10]$. The initial velocity is zero everywhere and the initial density satisfies $\rho = \bar{\rho}\left(\dfrac{p + p_\infty}{\bar{p} + p_\infty}\right)^{\frac{1}{\gamma}}$. For the 3×3 model k is also zero.

Riemann problem for multi-fluid

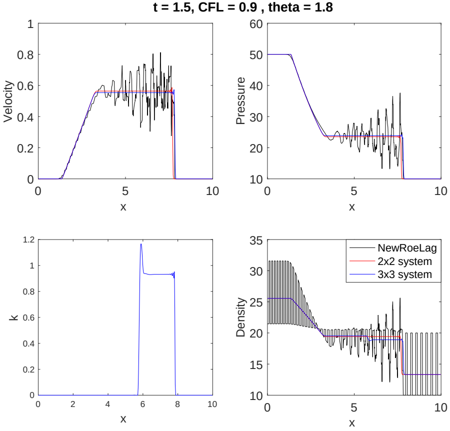

Figure: Comparison between detailed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.5$.

Riemann problem for multi-fluid

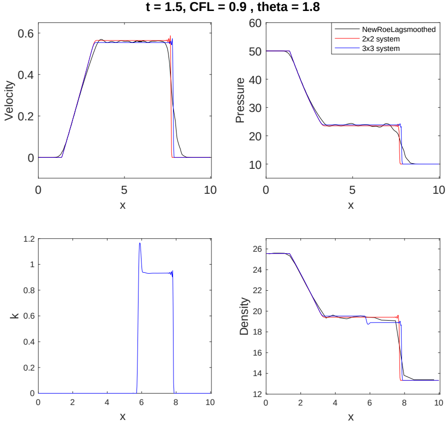

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 1.5$.

Riemann problem for multi-fluid

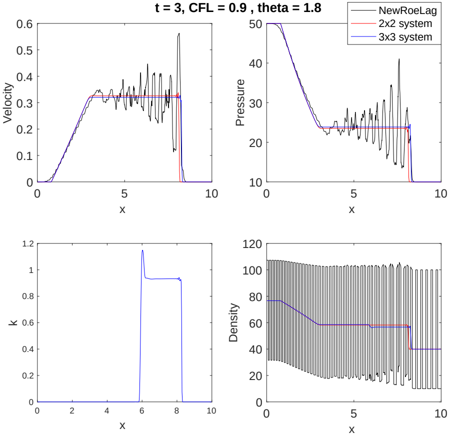

Figure: Comparison between detailed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 3$.

Riemann problem for multi-fluid

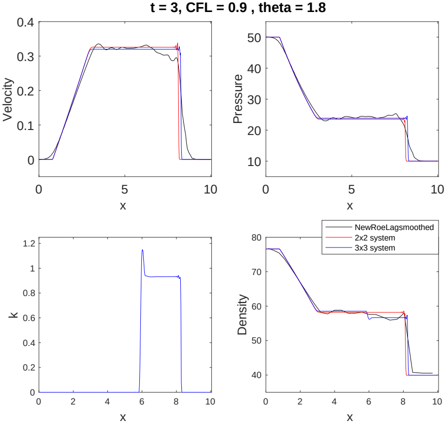

Figure: Comparison between smoothed numerical solution of multi-fluid and homogeneous models of Riemann problem (5.2) for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 3$.

Travelling shock - moderate density ratio

The initial condition of the travelling shock for 2×2 system is

$$\begin{cases} p_L = 40, u_L = 0.9452, & \text{if } 0 \leq x \leq 1 \\ p_R = 10, u_R = 0, & \text{if } 1 < x \leq 10, \end{cases} \tag{5.3}$$

and the initial density satisfies $\rho = \bar{\rho}\Big(\dfrac{p + p_\infty}{\bar{p} + p_\infty}\Big)^{\frac{1}{\gamma}}$.
At $x = 10$ we impose wall conditions : $u = 0$, $\partial p / \partial \xi = 0$.

Numerical results before hitting the wall

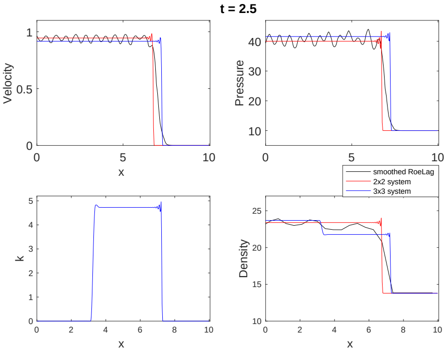

Figure: Comparison between smoothed detailed numerical solution, 2×2 system, 3×3 system before hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 2.5$.

Numerical results after hitting the wall

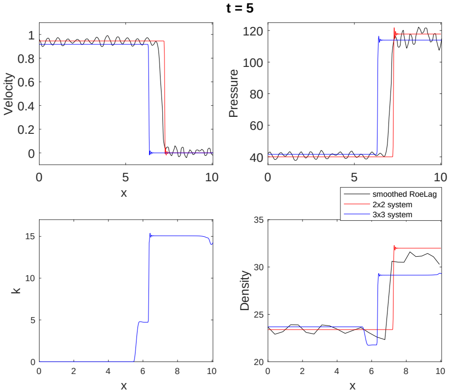

Figure: Comparison between smoothed detailed numerical solution, 2×2 system, 3×3 system after hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 2$ at time $t = 5$.

Travelling shock - big density ratio

The initial condition of the Riemann problem is

$$\begin{cases} p_L = 40, u_L = 0.5286, & \text{if } x \leq 1 \\ p_R = 10, u_R = 0, & \text{if } x > 1, \end{cases} \tag{5.4}$$

where $x \in [0, 10]$.

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

Numerical results before hitting the wall

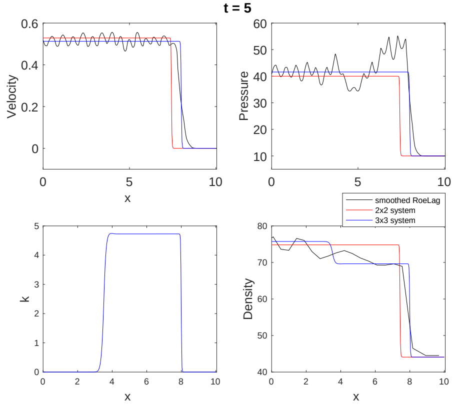

Figure: Comparison between smoothed detailed numerical solution, 2×2 system, 3×3 system before hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 5$.

Numerical results after hitting the wall

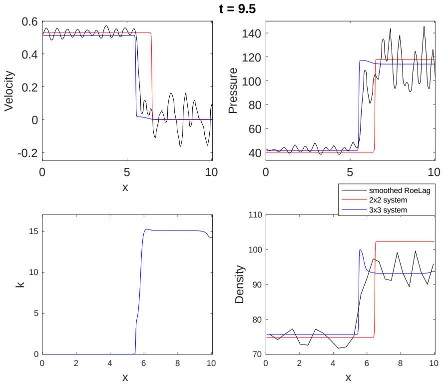

Figure: Comparison between smoothed detailed numerical solution, 2×2 system, 3×3 system after hitting the wall for the case of density ratio $\rho_{10}/\rho_{20} = 10$ at time $t = 9.5$.

Comparison of the computation time

Detailed computation	2×2 system	3×3 system
298.8	42.8	50.1

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 2×2 model gives a better prediction of the shock position.
    - For large density ratio, the turbulent 3×3 model is in better agreement with a smoothed out version of the detailed numerical compared with the simple 2×2 model.
- Open problem: construction of non isentropic homogenized models.

Reference

D.T. M. Phan, S.L. Gavrilyuk and G. Russo, "Numerical validation of homogeneous multi-fluid models", Applied Mathematics and Computation 441 (2023) 127693 https://doi.org/10.1016/j.amc.2022.127693

Thank you for your attention!