M.Sc. Simulation Sciences, Winter Semester 2016 / 2017

Numerical Methods for PDE

Prof. Georg May

Homework 6: The Shocktube problem

Due: Tuesday, January 17, 2017 (by Midnight)

1 Rules

This project is worth as much as two regular homeworks (20 points).

2 Problem Description

We consider inviscid, 1D compressible fluid flow. The governing equations, the Euler equations, are written as follows:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0 \ , \tag{1}$$

where

$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} \ , \qquad \mathbf{f} = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E+p) \end{pmatrix} \ . \tag{2}$$

Here, ρ is the density, u is the velocity, E is the energy, and p is the pressure. These are the equations we solve.

To determine the pressure, and close the equations, we need an equation of state. Here we use the ideal gas law in the following form:

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho u^2\right) \ , \tag{3}$$

where $\gamma = 1.4$ (physical constant).

3 Discretization

We discretize the equations using a finite volume method. We write for an arbitrary cell i:

$$\frac{d\mathbf{u}_i}{dt} + \frac{1}{\Delta x}\left(\hat{\mathbf{f}}_{i+\frac{1}{2}} - \hat{\mathbf{f}}_{i-\frac{1}{2}}\right) = 0 \ . \tag{4}$$

For simplicity we take a constant cell width: $\Delta x = const$. The most important ingredient of the numerical discretization is the numerical flux $\hat{\mathbf{f}}_{i+\frac{1}{2}}$. We consider two different formulations:

$$\hat{\mathbf{f}}_{i+\frac{1}{2}} = \frac{1}{2}\left(\mathbf{f}(\mathbf{u}_{i+1}) + \mathbf{f}(\mathbf{u}_i)\right) - \frac{\alpha_{i+\frac{1}{2}}}{2}\left(\mathbf{u}_{i+1} - \mathbf{u}_i\right) \ , \tag{5}$$

$$\hat{\mathbf{f}}_{i+\frac{1}{2}} = \frac{1}{2}\left(\mathbf{f}(\mathbf{u}_{i+1}) + \mathbf{f}(\mathbf{u}_i)\right) - \frac{1}{2}C^{Roe}|A^{Roe}_{i+\frac{1}{2}}|\left(\mathbf{u}_{i+1} - \mathbf{u}_i\right) \tag{6}$$

The scalar coefficient α is given by

$$\alpha_{i+\frac{1}{2}} = C \max(|u_i| + c_i, |u_{i+1}| + c_{i+1}) \; . \tag{7}$$

while the diffusion matrix A^{Roe} will be given below. The speed of sound c may be computed as

$$c_i = \sqrt{\gamma p_i / \rho_i} \tag{8}$$

The constants C, C^{Roe} can be used for fine tuning, where $C \approx C^{Roe} \approx 1$. You can experiment with the value a little when you do computations.

Define the enthalpy h as

$$h = \frac{E + p}{\rho}, \tag{9}$$

and define an averaging procedure for velocity and enthalpy:

$$\hat{u}_{i+\frac{1}{2}} = \frac{\sqrt{\rho_i} u_i + \sqrt{\rho_{i+1}} u_{i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}} \; , \tag{10}$$

$$\hat{h}_{i+\frac{1}{2}} = \frac{\sqrt{\rho_i} h_i + \sqrt{\rho_{i+1}} h_{i+1}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}} \; . \tag{11}$$

Using these particular averages we may compute the speed of sound as[1]

$$\hat{c}_{i+\frac{1}{2}} = \sqrt{(\gamma - 1)\left(\hat{h}_{i+\frac{1}{2}} - \frac{1}{2}\hat{u}^2_{i+\frac{1}{2}}\right)} \; . \tag{12}$$

We only need these three quantities to evaluate the matrix A^{Roe}. We omit subscripts and superscripts of averaged quantities from here on. However, we use only these averaged values when evaluating A^{Roe}! We write

$$|A^{Roe}_{i+\frac{1}{2}}| = R|\Lambda|R^{-1} \tag{13}$$

where $|\Lambda|$ where Λ is the diagonal matrix of eigenvalues.

$$|\Lambda| = \operatorname{diag}\{|\lambda_1|, |\lambda_2|, |\lambda_3|\} = \operatorname{diag}\{|u - c|, |u|, |u + c|\} \tag{14}$$

The matrix of eigenvectors is written

$$R = \begin{pmatrix} 1 & 1 & 1 \\ u - c & u & u + c \\ h - uc & \frac{1}{2}u^2 & h + uc \end{pmatrix} , \qquad R^{-1} = \begin{pmatrix} \frac{1}{2}\left(1 + \Gamma(u^2 - h) + \frac{u}{c}\right) & -\frac{1}{2}\left(\Gamma u + \frac{1}{c}\right) & \frac{1}{2}\Gamma \\ -\Gamma(u^2 - h) & \Gamma u & -\Gamma \\ \frac{1}{2}\left(1 + \Gamma(u^2 - h) - \frac{u}{c}\right) & -\frac{1}{2}\left(\Gamma u - \frac{1}{c}\right) & \frac{1}{2}\Gamma \end{pmatrix} , \tag{15}$$

where $\Gamma = (\gamma - 1)/c^2$. Using this decomposition the diffusion terms $A^{Roe}(\mathbf{u}_{i+1} - \mathbf{u}_i)$ are best evaluated as repeated matrix-vector products.

For discontinuous solutions one should replace the eigenvalues in (14) with $\widetilde{\lambda}_i$,

$$\widetilde{\lambda}_i = \begin{cases} \frac{1}{2}\left(A + \frac{\lambda_i^2}{A}\right) & \lambda_i < A \\ \lambda_i & otherwise \end{cases} , \qquad A = A_\lambda c \; , \tag{16}$$

where we take $A_\lambda = 1$. (c is again the Roe-averaged speed of sound.) This is called entropy fix, although we shall not elaborate on this here.

[1] Note that we compute the speed of sound differently, compared to (8), because we use the particular averages of u and h. both definitions of the speed of sound are equivalent, though.

For the time discretization we choose for the sake of simplicity a simple forward Euler explicit method:

$$\frac{\partial \mathbf{u}}{\partial t} \approx \frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\tau^n} \tag{17}$$

The discrete time step is set as

$$\tau^n = \mathrm{CFL}\frac{\Delta x}{\lambda^n_{max}} \tag{18}$$

where $\lambda^n_{max} = \max_i(|u^n_i| + c^n_i)$, and the maximum is taken over all cells. One controls the time step via the CFL number, which is of order unity.

4 Initial conditions

At time $t = 0$, we set the flow variables to [2]

$$\rho(0) = \begin{cases} 1 & x < \frac{1}{2} \\ 0.125 & x \geq \frac{1}{2} \end{cases}, \qquad E(0) = \begin{cases} 2.5 & x < \frac{1}{2} \\ 0.25 & x \geq \frac{1}{2} \end{cases}, \qquad u(0) = 0 \tag{19}$$

to initialize the flow field. This means

$$\mathbf{u}(0) = \begin{pmatrix} \rho(0) \\ \rho(0)u(0) \\ E(0) \end{pmatrix} \tag{20}$$

With these initial conditions, a characteristic pattern of expansion waves and discontinuities will be observed for the flow variables. Figure 1 shows an example for the density.

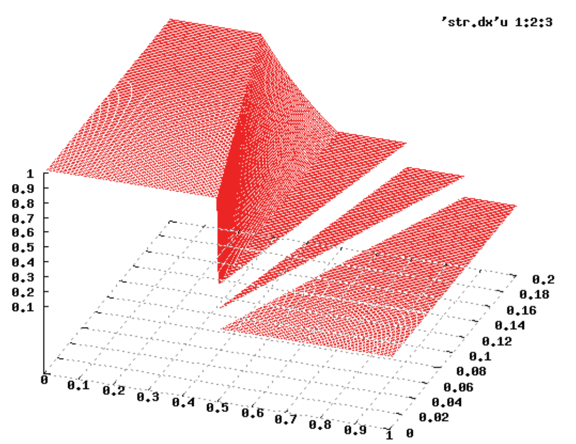

Figure 1: Time evolution of the density for the shock tube problem.(Density plotted against $x \in [0, 1]$ and $t \in [0, 0.2]$.) Initially, only one discontinuity is present. Subsequently, an expansion wave travels to the left, while two discontinuities travel to the right.

[2]Note: The variables are not given in physical units. We may think of the them as non-dimensionalized variables.

5 Boundary Conditions

The initial conditions define the shock-tube problem. The discontinuity at time $t = 0$ will cause shock waves and expansion fans to develop and propagate through the domain. We will not iterate in time long enough for these disturbances to reach the boundaries. Hence we may freeze the flow variables to constant values there.[3] Evaluate the boundary fluxes as discussd in class, i.e use $\mathbf{f}(\mathbf{u}(0))$ instead of $\mathbf{F}_{i\pm\frac{1}{2}}$ there.

6 Test Runs

Use a physical domain with $x \in [0, 1]$. Use two different grids: One with $N = 100$ points, and one with $N = 1,000$ points. Iterate in time for $t \in [0, T]$ where we set $T = 0.2$. Plot the density, the velocity, and the pressure against x, for the final time T. Do this for both choices of the flux. (Overplot the solution for both grids)

7 Instructions

In this section you find a crude outline of a possible implementation of the problem. It is recommend to structure the program such that it is divided into smaller modules. This can be roughly organized a follows:

- <u>initialization</u>: Initialize the flowfield via eq. (20).
- for $n = 1, 2, \ldots$
  - <u>time step</u>: Calculate the factor $\lambda_{\max}$, and set the time step according to eq. (18).
  - <u>fluxes</u>: Calculate fluxes in eq. (4) for all cells. Make sure that for the fluxes both eq. (5) (6) can be used.
  - <u>update</u>: Calculate the solution at the next time level using eq. (17). The pressure needs to be updated using the equation of state (3).
- <u>output</u>: Write out flow variables (Density, Mach number, Pressure, etc.)

[3]Note: Freezing the boundaries is in general not the proper way to set boundary conditions for hyperbolic systems. Here we get away with it, because the flow solution will remain constant near the boundaries.