ME 702 — COMPUTATIONAL FLUID DYNAMICS

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Practical Module — Sod's Test Problems

[Refs] 1) Sod, 1978. J. Comp. Phys., Vol 27: 1–31
2) C. Laney, 1998. "Computational Gas Dynamics", Cambridge Uni. Pre

TEST 1 Find the pressure, velocity, speed of sound, density, entropy and Mach number at $t = 0.01$ s, where

$$\underline{w}(x,0) = \begin{cases} \underline{w}_L & x < 0 \\ \underline{w}_R & x \geq 0 \end{cases}$$ corresponds to the initial conditions...

... using the vector notation of the Euler equation but in primitive variables:

$$\underline{w}_L = \begin{bmatrix} \rho_L \\ u_L \\ p_L \end{bmatrix} = \begin{bmatrix} 1 \ \mathrm{kg/m^3} \\ 0 \ \mathrm{m/s} \\ 100 \ \mathrm{kN/m^2} \end{bmatrix}$$

$$\underline{w}_R = \begin{bmatrix} \rho_R \\ u_R \\ p_R \end{bmatrix} = \begin{bmatrix} 0.125 \ \mathrm{kg/m^3} \\ 0 \ \mathrm{m/s} \\ 10 \ \mathrm{kN/m^2} \end{bmatrix}$$

Discretization: $N = 50$ points in $[-10\,\mathrm{m}, 10\,\mathrm{m}]$

$$\Delta x = \frac{20\,\mathrm{m}}{50} = 0.4\ \mathrm{m}$$, initial CFL = 0.4

Initial maximum wave speed = 374.17 m/s

Time step $$\Delta t = 0.4\left(\frac{0.4\ \mathrm{m}}{374.17\ \mathrm{m/s}}\right) = 4.276 \times 10^{-4}\ \mathrm{s}$$

$$\frac{\Delta t}{\Delta x} = 1.069 \times 10^{-3}\ \frac{\mathrm{s}}{\mathrm{m}}$$. The final time is thus reached in approximately 23 steps.

TEST 2 : Unknowns, same as Test 1.

$$\underline{w}_L = \begin{bmatrix} \rho_L \\ u_L \\ p_L \end{bmatrix} = \begin{bmatrix} 1 \ \ kg/m^3 \\ 0 \ \ m/s \\ 100 \ \ kN/m^2 \end{bmatrix}$$

$$\underline{w}_R = \begin{bmatrix} \rho_R \\ u_R \\ p_R \end{bmatrix} = \begin{bmatrix} 0.010 \ \ kg/m^3 \\ 0 \ \ m/s \\ 1 \ \ kN/m^2 \end{bmatrix}$$

Discretization $N = 50$ points in $[-10\text{ m}, 15\text{ m}]$

$$\Delta x = \frac{25\text{ m}}{50} = 0.5\text{ m}$$

initial CFL number $= 0.3$. Maximum initial wave speed $= 374.17 \frac{m}{s}$

$$\frac{\Delta t}{\Delta x} = 8.02 \times 10^{-4} \ \frac{s}{m}$$

Final time of $T = 0.01$ s is reached in approximately 25 time steps.

NOTES

- One must choose between fixing the maximum CFL number or fixing the time step (as the solution progresses, there can be faster waves than the initial condition, causing the CFL number to increase)
- In this practical module, the time step is fixed, for a more meaningful comparison among methods.
  In general circumstances, one would sensibly take the largest time step possible, consistent with accuracy & stability (i.e. fix CFL)
- When fixing Δt, one should be careful with overshoots in the wave speed which may violate the CFL condition
- Another problem is undershoots in pressure or density which may make them negative. One can replace negative values, e.g., making $p = \max(0, p)$.

The primitive variable form of the Euler equations

(commonly used for incompressible, viscous flow; less often used in compressible aerodynamics)

- Vector of primitive variables: $\underline{w} = \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}$
- Vector form of Euler eqns:

$$\boxed{\frac{\partial \underline{w}}{\partial t} + C \frac{\partial \underline{w}}{\partial x} = 0}$$

where

$$C = \begin{bmatrix} u & \rho & 0 \\ 0 & u & 1/\rho \\ 0 & \rho a^2 & u \end{bmatrix}$$

(unlike the matrix A in the conservai form, the matrix C in primitive variable form is not the Jacobia of any flux function)

a: speed of sound

$$a^2 = \gamma R T = \frac{\gamma p}{\rho} \quad \text{with} \quad \gamma = \frac{c_p}{c_v}$$

Using the material derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial x}$

the equations are:

1) $\frac{D\rho}{Dt} + \rho \frac{\partial u}{\partial x} = 0$ conservation of mass

2) $\frac{Du}{Dt} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0$ conservation of momentum

3) $\frac{Dp}{Dt} + \rho a^2 \frac{\partial u}{\partial x} = 0$ conservation of energy

4) $\frac{Ds}{Dt} \geqslant 0$ 2nd law of thermodynamics

* Primitive variables are those flow variables that are measured

The conservative formulation of the Euler equations

– For smooth solutions, both formulations are equivalent. But for solutions containing shocks, non-conservative formulations give incorrect shock solutions

- Vector of conserved variables $\underline{u} = \begin{bmatrix} \rho \\ \rho u \\ \rho e_T \end{bmatrix}$

  where $e_T = e + \frac{u^2}{2}$

  is the specific total energy.

- Vector form of Euler equations: $\boxed{\frac{\partial}{\partial t}\underline{u} + \frac{\partial}{\partial t}\underline{f} = 0}$

  with $\underline{f}$ the flux vector:

$$\underline{f} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_T + p)u \end{bmatrix} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho h_T u \end{bmatrix}$$

  where in the second version we use the enthalpy (total)

$$h_T = e_T + p/\rho = h + u^2/2$$

- Using the Jacobian matrix, the Euler equations are written in quasi-linear form: $\boxed{\frac{\partial}{\partial t}\underline{u} + A\frac{\partial}{\partial x}\underline{u} = 0}$

$$A(\underline{u}) = \frac{\partial \vec{F}}{\partial \underline{u}} = \begin{bmatrix} \partial f_1/\partial u_1 & \partial f_1/\partial u_2 & \partial f_1/\partial u_3 \\ \partial f_2/\partial u_1 & \partial f_2/\partial u_2 & \partial f_2/\partial u_3 \\ \partial f_3/\partial u_1 & \partial f_3/\partial u_2 & \partial f_3/\partial u_3 \end{bmatrix}$$

To obtain the Jacobian matrix, first express the flux components f_i in terms of the components of $\underline{u}$

Euler Jacobian matrix

flux: $\underline{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ u(\rho e_T + p) \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$

So: $f_1 = \rho u = u_2$

For f_2 and f_3 $\rightarrow$ need p in terms of conserved variables

$e_T = e + \frac{1}{2}u^2$ so $f_3 = [\rho(e + \frac{1}{2}u^2) + p]\, u$

Equation of State for ideal gases: $e = e(\rho, p) = \dfrac{p}{(\gamma-1)\rho}$, $\gamma = 1.4$

$$\rightarrow p = (\gamma - 1)\rho \cdot e$$

$$p = (\gamma-1)\Big(\underbrace{\rho e_T}_{u_3} - \underbrace{\rho u^2/2}_{\frac{1}{2}\cdot u_2^2/u_1}\Big) = (\gamma-1)\left(u_3 - \frac{1}{2}\frac{u_2^2}{u_1}\right)$$

So, the flux vector is:

$$\underline{F} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} u_2 \\ u_2^2/u_1 + (\gamma-1)\left(u_3 - \frac{u_2^2}{2u_1}\right) \\ \left(u_3 + (\gamma-1)\left(u_3 - \frac{u_2^2}{2u_1}\right)\right)\frac{u_2}{u_1} \end{bmatrix}$$

rearranging:

$$f_2 = (3-\gamma)\frac{u_2^2}{2u_1} + (\gamma-1)u_3$$

$$f_3 = \gamma \cdot \frac{u_2}{u_1} \cdot u_3 - \frac{(\gamma-1)}{2}\frac{u_2^3}{u_1^2}$$

Taking all derivatives, the Jacobian matrix is obtained;

$$A(\underline{u}) = \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2}(\gamma-3)\left(\frac{u_2}{u_1}\right)^2 & (3-\gamma)\frac{u_2}{u_1} & \gamma-1 \\ -\gamma\frac{u_2 u_3}{u_1^2} + (\gamma-1)\left(\frac{u_2}{u_1}\right)^3 & \gamma\frac{u_3}{u_1} - \frac{3}{2}(\gamma-1)\left(\frac{u_2}{u_1}\right)^2 & \gamma\frac{u_2}{u_1} \end{bmatrix}$$

The Jacobian matrix is written in terms of the sound speed, a and the velocity

$$A(\underline{u}) = \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2}(\gamma-3)u^2 & (3-\gamma)u & \gamma-1 \\ \frac{1}{2}(\gamma-2)u^3 - \frac{a^2 u}{\gamma-1} & \frac{3-2\gamma}{2}u^2 + \frac{a^2}{\gamma-1} & \gamma u \end{bmatrix}$$

Discretizing the Euler equations

1) Lax-Friedrichs scheme (1st order)

$$\underline{u}_i^{n+1} = \frac{1}{2}\left(\underline{u}_{i+1}^n + \underline{u}_{i-1}^n\right) - \frac{\Delta t}{2\Delta x}\left[\underline{f}(\underline{u}_{i+1}^n) - \underline{f}(\underline{u}_{i-1}^n)\right]$$

2) Lax-Wendroff scheme (2nd order)

$$\underline{u}_i^{n+1} = \underline{u}_i^n - \frac{\Delta t}{2\Delta x}\left[\underline{f}_{i+1}^n - \underline{f}_{i-1}^n\right] + \dots$$

$$+ \frac{\Delta t^2}{2\Delta x^2}\left[A_{i+1/2}^n\left(\underline{f}_{i+1}^n - \underline{f}_i^n\right) - A_{i-1/2}^n\left(\underline{f}_i^n - \underline{f}_{i-1}^n\right)\right]$$

with, e.g.

$$A_{i+1/2}^n = A\left(\frac{\underline{u}_{i+1}^n + \underline{u}_i^n}{2}\right)$$

3) Richtmyer method

$$\underline{u}_{i+1/2}^{n+1/2} = \frac{1}{2}\left(\underline{u}_{i+1}^n + \underline{u}_i^n\right) - \frac{\Delta t}{2\Delta x}\left(\underline{f}_{i+1}^n - \underline{f}_i^n\right)$$

$$\underline{u}_i^{n+1} = \underline{u}_i^n - \frac{\Delta t}{\Delta x}\left(\underline{f}_{i+1/2}^{n+1/2} - \underline{f}_{i-1/2}^{n+1/2}\right)$$

4) MacCormack method

$$\underline{u}_i^{*} = \underline{u}_i^{n} - \frac{\Delta t}{\Delta x}\left(\underline{f}_{i+1}^{n} - \underline{f}_i^{n}\right)$$

$$\underline{u}_i^{n+1} = \frac{1}{2}\left(\underline{u}_i^{n} + \underline{u}_i^{*}\right) - \frac{\Delta t}{2\Delta x}\left(\underline{f}_i^{*} - \underline{f}_{i-1}^{*}\right)$$

Assignment

* Solve the two test problems using

- Lax-Friedrichs
- Lax-Wendroff
- Richtmyer
- MacCormack

with and without artificial dissipation

Artificial dissipation (2nd order)

$$\epsilon\left(\underline{u}_{i+1}^{n} - 2\underline{u}_i^{n} + \underline{u}_{i-1}^{n}\right)$$

- add to 1st step of MacCormack & 2nd step of Richtmyer

* $\underline{u}$ must be "decoded" to obtain the primitive variables for plotting of the solution