AE/ME 339
Computational Fluid Dynamics (CFD)

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MacCormack's Second-Order Accurate Two-Step Method

MacCormack's method (6.3)
Summary of steps

- Original (1969) method is 2nd order accurate (in space and time), explicit method
- It is a modified form of the Lax-Wendroff scheme (6.2)
- The method has a predictor step and a corrector step
- An average value of the time derivative is first calculated
- Solution is advanced to the next time level using the average value of the time derivative
- Average value of the time derivative are calculated by using a predictor step and a corrector step
- Both forward and backward differences are used for space derivatives in calculating the average value of the time derivative, the reason for second order accuracy

MacCormack's method (6.3)

The following expression shows how density for the next time level is calculated using the calculated average value of the derivative

$$\rho_i^{n+1} = \rho_i^n + \left(\frac{\partial \rho}{\partial t}\right)_{avg} \Delta t ....(6.13)$$

Predictor step (using forward difference for space derivative)

$$\left(\frac{\partial \rho}{\partial t}\right)_i^n = -\left(\rho_i^n \frac{u_{i+1}^n - u_i^n}{\Delta x} + u_i^n \frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\right)...(6.17)$$

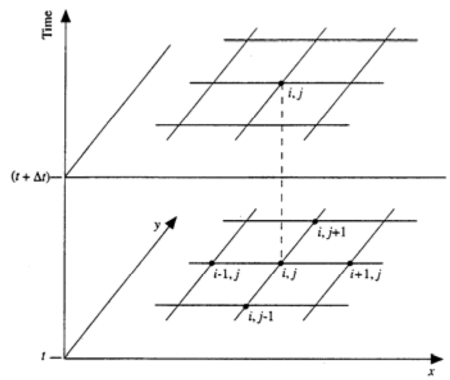

Figure 6.2

Predicted value, first order accurate. (Note that the overbar here corresponds to the predictor step. It is different from its meaning in Eq. (2.93) where it denotes a column vector.)

$$\bar{\rho}_i^{n+1} = \rho_i^n + \left(\frac{\partial \rho}{\partial t}\right)_i^n \Delta t ....(6.18)$$

Similar equations can be written for the predicted values of the other variables in the U_bar vector (recall the matrix representation of the equations.

Note that the forward difference is used in Eq. (6.17) for the space derivative

Now obtain a corrected value of the time derivative using backward difference for the space derivatives. (Note use of backward difference for space derivative in equation below.)

$$\left(\frac{\overline{\partial\rho}}{\partial t}\right)_i^{n+1} = -\left(\overline{\rho}_i^{n+1}\frac{\overline{u}_i^{n+1}-\overline{u}_{i-1}^{n+1}}{\Delta x}+\overline{u}_i^{n+1}\frac{\overline{\rho}_i^{n+1}-\overline{\rho}_{i-1}^{n+1}}{\Delta x}\right) \text{...(6.21)}$$

Now find average value of the time derivative as

$$\left(\frac{\partial\rho}{\partial t}\right)_{avg} = \frac{1}{2}\left[\left(\frac{\partial\rho}{\partial t}\right)_{i,j}^{n} + \left(\frac{\overline{\partial\rho}}{\partial t}\right)_{i,j}^{n+1}\right] \text{.........(6.22)}$$

Now use Eq. (6.13) to calculate the variable at (n+1)

$$\rho_i^{n+1} = \rho_i^n + \left(\frac{\partial\rho}{\partial t}\right)_{avg}\Delta t \text{.........(6.13)}$$

Repeat the procedure to get the variable at all the grid points shown
In Figure 6.2

The same procedure can be used for all the other variables of the solution vector U_bar, using forward difference for the predictor step and backward difference for the corrector step.

Because of using forward difference for the predictor and backward differnce for the corrector steps, the method can be shown to be 2nd order accurate.

Implementation for shock tube problem

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The Shock Tube Process (11.4.2)

Insert Figure 11.5

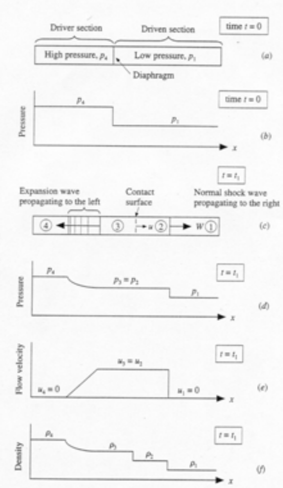

FIG. 11.5

Wave structure in shock
Tube process

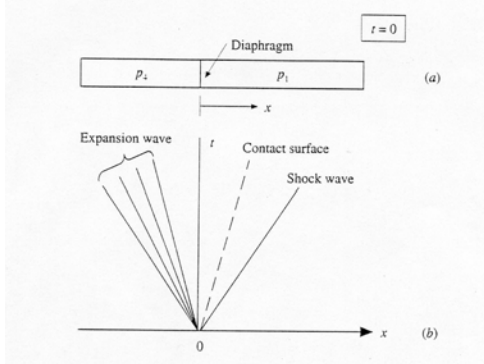

Figure 11.6

Consists of a high pressure chamber and a low pressure chamber separated by a diaphragm

When the diaphragm is broken a wave pattern is established as shown In the figure

Figure shows the flow at a certain time t1, when the waves haven’t Started reflecting from the tube ends

Recall the following vector form of the equations

$$\frac{\partial \bar{U}}{\partial t}+\frac{\partial \bar{F}}{\partial x}+\frac{\partial \bar{G}}{\partial y}+\frac{\partial \bar{H}}{\partial z}=\bar{J} \quad \text{..................(2.93)}$$

$$\bar{U}=\left\{\begin{matrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho\left(e+\frac{V^2}{2}\right) \end{matrix}\right\} \quad \text{............(2.94)}$$

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$$\bar{F}=\left\{\begin{matrix} \rho u \\ \rho u^2+p-\tau_{xx} \\ \rho \mathrm{v} u-\tau_{xy} \\ \rho w u-\tau_{xz} \\ \rho\left(e+\frac{V^2}{2}\right)u+pu-k\frac{\partial T}{\partial x}-u\tau_{xx}-\mathrm{v}\tau_{xy}-w\tau_{xz} \end{matrix}\right\} \quad (2.95)$$

$$\bar{G} = \begin{Bmatrix} \rho v \\ \rho uv - \tau_{yx} \\ \rho v^2 + p - \tau_{yy} \\ \rho wv - \tau_{yz} \\ \rho\left(e + \frac{V^2}{2}\right)v + pv - k\frac{\partial T}{\partial y} - u\tau_{yx} - v\tau_{yy} - w\tau_{yz} \end{Bmatrix} \quad (2.96)$$

$$\bar{H} = \begin{Bmatrix} \rho w \\ \rho uw - \tau_{zx} \\ \rho vw - \tau_{zy} \\ \rho w^2 + p - \tau_{zz} \\ \rho\left(e + \frac{V^2}{2}\right)w + pw - k\frac{\partial T}{\partial z} - u\tau_{zx} - v\tau_{zy} - w\tau_{zz} \end{Bmatrix} \quad (2.97)$$

$$\bar{J} = \begin{Bmatrix} 0 \\ \rho f_x \\ \rho f_y \\ \rho f_z \\ \rho\left(uf_x + vf_y + wf_z\right) + \rho\dot{q} \end{Bmatrix} \quad (2.98)$$

The above vectors can be modified for the shock tube problem. Since only one space dimension is present, the vectors can be shortened as follows

$$\frac{\partial \bar{U}}{\partial t} + \frac{\partial \bar{F}}{\partial x} = \bar{J} \text{..................}(A)$$

$$\bar{U} = \begin{Bmatrix} \rho \\ \rho u \\ \rho\left(e + \frac{u^2}{2}\right) \end{Bmatrix} \text{...........}(B)$$

$$\bar{F} = \begin{Bmatrix} \rho u \\ \rho u^2 + p - \tau_{xx} \\ \rho\left(e + \frac{u^2}{2}\right) u + pu - k\frac{\partial T}{\partial x} - u\tau_{xx} \end{Bmatrix} \text{................}(C)$$

$$\bar{J} = \begin{Bmatrix} 0 \\ 0 \\ \rho \dot{q} \end{Bmatrix} \text{...............}(D)$$

$$U_1 = \rho$$
$$U_2 = \rho u$$
$$U_3 = \rho(c_v T + \frac{u^2}{2})$$
$$u = U_2 / U_1$$
$$U_3 = U_1(c_v T + \frac{u^2}{2})$$

$$c_v T + \frac{u^2}{2} = \frac{U_3}{U_1}$$
$$T = \frac{1}{c_v}\left(\frac{U_3}{U_1} - \frac{u^2}{2}\right)$$
$$F_1 = \rho u$$
$$F_2 = \rho u^2 + p - \tau_{xx}$$
$$F_3 = \rho u(e + \frac{u^2}{2}) + pu - k\frac{\partial T}{\partial x} - u\tau_{xx}$$

Recall that, according to Stokes hypothesis $\lambda = -(2/3)\mu$

Also recall that

$$\tau_{xx} = \lambda \overline{\nabla} \cdot \overline{V} + 2\mu \frac{\partial u}{\partial x} = -\frac{2}{3}\mu \frac{\partial u}{\partial x} + 2\mu \frac{\partial u}{\partial x} = \frac{4}{3}\mu \frac{\partial u}{\partial x}$$

Therefore

$$F_2 = \rho u^2 + p - \frac{4}{3}\mu \frac{\partial u}{\partial x}$$

Also note

$$F_1 = U_2$$

If we neglect external heating, the J-vector on the RHS will be = 0. Therefore we can write

vector form: $$\frac{\partial \overline{U}}{\partial t} = -\frac{\partial \overline{F}}{\partial x}$$

Continuity: $$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(\rho u)$$

Momentum: $$\frac{\partial (\rho u)}{\partial t} = -\frac{\partial}{\partial x}\left[\rho u^2 + p - \frac{4}{3}\mu \frac{\partial u}{\partial x}\right]$$

Energy:

$$\frac{\partial}{\partial t}\left[\rho(e + \frac{u^2}{2})\right] = -\frac{\partial}{\partial x}\left[\rho u(e + \frac{u^2}{2}) + pu - k\frac{\partial T}{\partial x} - \frac{4}{3}\mu u \frac{\partial u}{\partial x}\right]$$

Auxiliary relations for a perfect gas

$$p = \rho R T$$
$$e = c_v T$$
$$h = c_p T$$

First calcuate $\overline{U}_i^{n+1}$ from the equation below

$$\frac{\overline{U}_i^{n+1} - U_i^n}{\Delta t} = -\frac{F_{i+1}^n - F_i^n}{\Delta x}$$

Next Calculate $\overline{F}^{n+1}$ from $\overline{U}^{n+1}$

Now calculate U_i^{n+1} from

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = -\frac{1}{2}\left[\frac{F_{i+1}^n - F_i^n}{\Delta x} + \frac{\overline{F}_i^{n+1} - \overline{F}_{i-1}^{n+1}}{\Delta x}\right]$$

$$\frac{U_i^{n+1}-U_i^n}{\Delta t}=-\frac{1}{2}\left[-\frac{\overline{U}_i^{n+1}-U_i^n}{\Delta t}+\frac{\overline{F}_i^{n+1}-\overline{F}_{i-1}^{n+1}}{\Delta x}\right]$$

$$U_i^{n+1}=U_i^n+\frac{1}{2}(\overline{U}_i^{n+1}-U_i^n)-\frac{\Delta t}{2\Delta x}(\overline{F}_i^{n+1}-\overline{F}_{i-1}^{n+1})$$

$$U_i^{n+1}=\frac{1}{2}(U_i^n+\overline{U}_i^{n+1})-\frac{\Delta t}{2\Delta x}(\overline{F}_i^{n+1}-\overline{F}_{i-1}^{n+1})$$

$$U_1=\rho$$

$$U_2=\rho u$$

$$U_3=\rho(c_vT+\frac{u^2}{2})$$

$$F_1=\rho u$$

$$F_2=\rho u^2+p-\frac{4}{3}\mu\frac{\partial u}{\partial x}$$

$$F_3=\rho u(c_vT+\frac{u^2}{2})+pu-\frac{4}{3}\mu u\frac{\partial u}{\partial x}$$

Note the axial conduction term in F_3 is neglected as it is small compared to the other terms

$$u = \frac{U_2}{U_1}$$

$$c_v T + \frac{u^2}{2} = \frac{U_3}{\rho}$$

$$T = \frac{U_3}{\rho c_v} - \frac{u^2}{2c_v} = \frac{1}{c_v}\left[\frac{U_3}{U_1} - \frac{1}{2}\frac{U_2^2}{U_1^2}\right] = \frac{1}{c_v U_1}\left[U_3 - \frac{1}{2}\frac{U_2^2}{U_1}\right]$$

$$p = \rho RT = U_1 R\left\{\frac{1}{c_v U_1}\left[U_3 - \frac{1}{2}\frac{U_2^2}{U_1}\right]\right\} = \frac{R}{c_v}\left[U_3 - \frac{1}{2}\frac{U_2^2}{U_1}\right]$$

$$F_1 = U_2$$

$$F_2 = u(\rho u) + p - \frac{4}{3}\mu\frac{\partial u}{\partial x}$$

$$F_2 = \frac{U_2}{U_1}U_2 + \frac{R}{c_v}U_3 - \frac{R}{2c_v}\frac{U_2^2}{U_1} - \frac{4}{3}\mu\frac{\partial u}{\partial x}$$

$$F_2 = \frac{R}{c_v}U_3 + \frac{U_2^2}{U_1}\left[1 - \frac{R}{2c_v}\right] - \frac{4}{3}\mu\frac{\partial u}{\partial x}$$

$$F_3 = U_2\left[\frac{c_p}{U_1 c_v}\left(U_3 - \frac{1}{2}\frac{U_2^2}{U_1}\right) + \frac{1}{2}\frac{U_2^2}{U_1^2}\right] - \frac{4}{3}\mu u\frac{\partial u}{\partial x}$$

The last terms in the momentum and energy equations that contain μ are the viscous dissipation terms.

The shock tube flow can be solved without including these terms (Euler form). However, the resulting numerical scheme will give rise to oscillations at sharp discontinuities such as the shock.

In order to avoid these oscillations, terms similar to the viscous terms are introduced to smear out the discontinuities.
These terms are sometimes called the "artificial viscosity term."

von Neumann and Richtmyer used a form of the artificial viscosity term which for the MacCormack scheme can be written as follows.

von Neumann-Richtmyer made the artificial viscosity term proportional to the velocity gradient as given below, where the proportionality constant, D, has the form shown on the RHS for the three equations.

$$D\frac{\partial u}{\partial x} = \underbrace{\alpha\left(\Delta x\right)^2 \rho \begin{vmatrix} 0 \\ 1 \\ u \end{vmatrix} \left|\frac{\partial u}{\partial x}\right|}_{D} \frac{\partial u}{\partial x}$$

Two corresponding finite difference forms are given below.

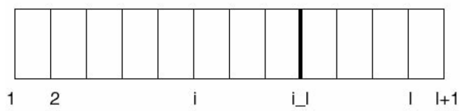
$$D_{i+\frac{1}{2}}(u_{i+1}-u_i)=\alpha\rho_{i+\frac{1}{2}}\begin{vmatrix}0\\1\\u\end{vmatrix}_{i+\frac{1}{2}}|u_{i+1}-u_i|(u_{i+1}-u_i)$$

$$D_{i+\frac{1}{2}}(u_{i+1}-u_i)=\alpha\rho_i\begin{vmatrix}0\\1\\u\end{vmatrix}_i|u_{i+1}-u_i|(u_{i+1}-u_i)$$

Note that D is a positive quantity. α is an empirical factor of $O(1)$ to be adjusted by closely monitoring the solution. α should be as small as possible and yet avoid oscillations.

$$\bar{U}_i^{n+1}=U_i^n-\frac{\Delta t}{\Delta x}(F_{i+1}^n-F_i^n)+$$
$$\frac{\Delta t}{\Delta x}\left[D^n_{i+\frac{1}{2}}(u^n_{i+1}-u^n_i)-D^n_{i-\frac{1}{2}}(u^n_i-u^n_{i-1})\right]$$

$$U_i^{n+1}=\frac{1}{2}(U_i^n+\bar{U}_i^{n+1})-\frac{\Delta t}{2\Delta x}(\bar{F}_i^{n+1}-\bar{F}_{i-1}^{n+1})+$$
$$\frac{\Delta t}{\Delta x}\left[\bar{D}_{i+\frac{1}{2}}(\bar{u}_{i+1}-\bar{u}_i)-\bar{D}_{i-\frac{1}{2}}(\bar{u}_i-\bar{u}_{i-1})\right]$$



Shock Tube Schematic

Initial conditions

$$u_i^n = 0 ....i = 1, I + 1$$

$$p_i^n = p_1 ....i = 1, i_l$$

$$p_i^n = p_2 ....i = i_l + 1, I + 1$$

$$T_i^n = T_0 ....i = 1, I + 1$$

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Boundary conditions
Wall at i = 1

set $u_1 = 0$

Open end (i = I+1)

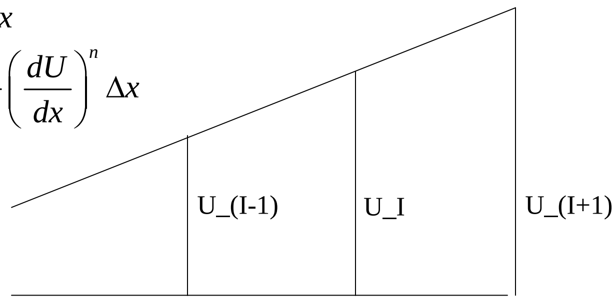
set $p_{I+1} = p_{amb}$

Other boundary conditions can be obtained by linear extrapolation

Extrapolation method for the right boundary

$$\frac{dU}{dx} = \frac{U_I - U_{I\_1}}{\Delta x}$$

$$U_{I+1}^{n+1} = U_I^n + \left(\frac{dU}{dx}\right)^n \Delta x$$



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Substitution gives

$$U_{I+1}^{n+1} = 2U_I^n - U_{I-1}^n$$

Similarly an expression can be written for the left boundary

$$\frac{dU}{dx} = \frac{U_3 - U_2}{\Delta x}$$

$$U_1 = U_2 - \frac{dU}{dx}\Delta x$$

$$U_1^{n+1} = 2U_2^n - U_3^n$$