AE/ME 339
Computational Fluid Dynamics (CFD)

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MacCormack’s method (6.3)

Original (1969) method is 2\textsuperscript{nd} order accurate (in space and time) explicit method. It is a modified form of the Lax-Wendroff scheme. Using MacCormack’s method we write

\[
\rho_{i,j}^{n+1} = \rho_{i,j}^n + \left( \frac{\partial \rho}{\partial t} \right)_{\text{avg}} \Delta t \ldots \ldots (6.13)
\]

Predictor step

\[
\left( \frac{\partial \rho}{\partial t} \right)_{i,j}^n = -\left( \rho_{i,j}^n \frac{u_{i+1,j}^n - u_{i,j}^n}{\Delta x} + u_{i,j}^n \frac{\rho_{i+1,j}^n - \rho_{i,j}^n}{\Delta x} \right) \ldots (6.17)
\]
Insert Figure 6.2
Predicted value, first order accurate

\[ \bar{\rho}_{i,j}^{n+1} = \rho_{i,j}^{n} + \left( \frac{\partial \rho}{\partial t} \right)_{i,j}^{n} \Delta t \quad \cdots \cdots (6.18) \]

Similar equations can be written for the predicted values of the Other variables in the U_bar vector.

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

First obtain a predicted value of the time derivative using backward difference for the space derivatives

\[
\left( \frac{\partial \rho}{\partial t} \right)_{i,j}^{n+1} = - \left( \frac{\bar{u}_{i,j}^{n+1} - \bar{u}_{i-1,j}^{n+1}}{\Delta x} \rho_{i,j}^{n+1} + \bar{u}_{i,j}^{n+1} \frac{\bar{\rho}_{i,j}^{n+1} - \bar{\rho}_{i-1,j}^{n+1}}{\Delta x} \right) \ldots (6.21)
\]

Now find average value of the time derivative as

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

\[
\left( \frac{\partial \rho}{\partial t} \right)_{avg} = \frac{1}{2} \left[ \left( \frac{\partial \rho}{\partial t} \right)_{i,j}^{n} + \left( \frac{\partial \rho}{\partial t} \right)_{i,j}^{n+1} \right] \ldots (6.22)
\]
Now use Eq. (6.13) to calculate the variable at (n+1)

\[
\rho_{i,j}^{n+1} = \rho_{i,j}^{n} + \left( \frac{\partial \rho}{\partial t} \right)_{avg} \Delta t \quad \ldots\ldots\ldots (6.13)
\]

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 difference for the corrector step, the method can be shown to be 2\textsuperscript{nd} order accurate.
The Shock Tube Process (11.4.2)

Insert Figure 11.5
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 \( t_1 \) when the waves haven’t started reflecting from the tube ends.

Insert Figure 11.6
Recall the following vector form of the equations

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

\[
\bar{U} = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho \left( e + \frac{V^2}{2} \right)
\end{bmatrix} \quad \text{.................}(2.94)
\]
\[ \bar{F} = \begin{cases} 
\rho u \\
\rho u^2 + p - \tau_{xx} \\
\rho vu - \tau_{xy} \\
\rho wu - \tau_{xz} \\
\rho \left( e + \frac{V^2}{2} \right) u + pu - k \frac{\partial T}{\partial x} - u\tau_{xx} - v\tau_{xy} - w\tau_{xz} 
\end{cases} \]............(2.95)
\[
\vec{G} = \left\{ \begin{array}{l}
\rho v \\
\rho u v - \tau_{yx} \\
\rho v^2 + p - \tau_{yy} \\
\rho w v - \tau_{yz} \\
\rho \left( e + \frac{V^2}{2} \right) w + p v - k \frac{\partial T}{\partial y} - u \tau_{yx} - v \tau_{yy} - w \tau_{yz} 
\end{array} \right\}
\]

\[
..................(2.96)
\]

\[
\vec{H} = \left\{ \begin{array}{l}
\rho w \\
\rho u w - \tau_{zx} \\
\rho v w - \tau_{zy} \\
\rho w^2 + p - \tau_{zz} \\
\rho \left( e + \frac{V^2}{2} \right) w + p w - k \frac{\partial T}{\partial z} - u \tau_{zx} - v \tau_{zy} - w \tau_{zz} 
\end{array} \right\}
\]

\[
..................(2.97)
\]
\[
\bar{J} = \begin{bmatrix}
0 \\
\rho f_x \\
\rho f_y \\
\rho f_z \\
\rho (u f_x + v f_y + w f_z) + \rho q
\end{bmatrix}
\] .........(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

\[
\frac{\partial \bar{U}}{\partial t} + \frac{\partial \bar{F}}{\partial x} = \bar{J} \tag{A}
\]

\[
\bar{U} = \begin{bmatrix}
\rho \\
\rho u \\
\rho \left( e + \frac{u^2}{2} \right)
\end{bmatrix} \tag{B}
\]
\[ \bar{E} = \begin{cases} 
\rho u \\
\rho u^2 + p - \tau_{xx} \\
\rho \left( e + \frac{u^2}{2} \right) u + pu - k \frac{\partial T}{\partial x} - u \tau_{xx} 
\end{cases} \] ........................(C)

\[ \bar{J} = \begin{cases} 
0 \\
0 \\
\rho \dot{q} 
\end{cases} \] ........................(D)
\[ U_1 = \rho \]
\[ U_2 = \rho u \]
\[ U_3 = \rho (c_v T + \frac{u^2}{2}) \]
\[ u = U_2 / U_1 \]
\[ U_3 = U_1 (c_v T + \frac{u^2}{2}) \]
\[ c_v T + \frac{u^2}{2} = \frac{U_3}{U_1} \]

\[ T = \frac{1}{c_v} \left( \frac{U_3}{U_1} - \frac{u^2}{2} \right) \]

\[ E_1 = \rho u \]

\[ E_2 = \rho u^2 + p - \tau_{xx} \]

\[ E_3 = \rho u \left( e + \frac{u^2}{2} \right) + pu + \dot{q}_x - u \tau_{xx} \]
Recall that, according to Stokes hypothesis $\lambda = -(2/3)\mu$

Also recall that

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

Therefore

$$
E_2 = \rho u^2 + p - \frac{4}{3} \mu \frac{\partial u}{\partial x}
$$

Also recall

$$
E_1 = U_2
$$
If we neglect external heating, the J-vector on the RHS will be $= 0$. Therefore we can write

$$\frac{\partial \bar{U}}{\partial t} = -\frac{\partial \bar{E}}{\partial x}$$

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

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

$$\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{u^2}{2} \right) \right] = -\frac{\partial}{\partial x} \left[ \rho u \left( e + \frac{u^2}{2} \right) + pu - \frac{4}{3} \mu u \frac{\partial u}{\partial x} \right]$$
Auxiliary relations for a perfect gas

\[ p = \rho RT \]
\[ e = c_v T \]
\[ h = c_p T \]
\[ \frac{\bar{U}_i^{n+1} - U_i^n}{\Delta t} = - \frac{E_{i+1}^n - E_i^n}{\Delta x} \]

Calculate \( \bar{E}^{n+1} \) from \( \bar{U}^{n+1} \)

\[ \frac{U_i^{n+1} - U_i^n}{\Delta t} = - \frac{1}{2} \left[ \frac{E_{i+1}^n - E_i^n}{\Delta x} + \frac{\bar{E}_{i+1}^{n+1} - \bar{E}_{i-1}^{n+1}}{\Delta x} \right] \]
\[
\frac{U_{i}^{n+1} - U_{i}^{n}}{\Delta t} = -\frac{1}{2} \left[ \frac{-\overline{U}_{i}^{n+1} - U_{i}^{n}}{\Delta t} + \frac{\overline{E}_{i}^{n+1} - \overline{E}_{i-1}^{n+1}}{\Delta x} \right] \\
U_{i}^{n+1} = U_{i}^{n} + \frac{1}{2} (\overline{U}_{i}^{n+1} - U_{i}^{n}) - \frac{\Delta t}{2\Delta x} (\overline{E}_{i}^{n+1} - \overline{E}_{i-1}^{n+1}) \\
U_{i}^{n+1} = \frac{1}{2} (U_{i}^{n} + \overline{U}_{i}^{n+1}) - \frac{\Delta t}{2\Delta x} (\overline{E}_{i}^{n+1} - \overline{E}_{i-1}^{n+1})
\]
\[ U_1 = \rho \]
\[ U_2 = \rho u \]
\[ U_3 = \rho(c_vT + \frac{u^2}{2}) \]
\[ E_1 = \rho u \]
\[ E_2 = \rho u^2 + p - \frac{4}{3} \mu \frac{\partial u}{\partial x} \]
\[ E_3 = \rho u(c_vT + \frac{u^2}{2}) + pu - \frac{4}{3} \mu u \frac{\partial u}{\partial x} \]
\[ u = \frac{U_2}{U_1} \]

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

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

\[ p = \rho RT = U_1 R \left\{ \frac{1}{c_v U_1} \left[ U_3 - \frac{1}{2} \frac{U_2^2}{U_1} \right] \right\} = \frac{R}{c_v} \left[ U_3 - \frac{1}{2} \frac{U_2^2}{U_1} \right] \]
\[ E_1 = U_2 \]

\[ E_2 = u(\rho u) + p - \frac{4}{3} \mu \frac{\partial u}{\partial x} \]

\[ E_2 = \frac{U_2}{U_1} U_2 + \frac{R}{c_v} U_3 - \frac{R}{2c_v} U_1^2 - \frac{4}{3} \mu \frac{\partial u}{\partial x} \]

\[ E_2 = \frac{R}{c_v} U_3 + \frac{U_2}{U_1} \left[ 1 - \frac{R}{2c_v} \right] - \frac{4}{3} \mu \frac{\partial u}{\partial x} \]

\[ E_3 = U_2 \left[ \frac{c_p}{U_1 c_v} \left( U_3 - \frac{1}{2} \frac{U_2^2}{U_1} \right) + \frac{1}{2} \frac{U_2^2}{U_1^2} \right] - \frac{4}{3} \mu u \frac{\partial u}{\partial x} \]