Implementing a Real-Gas Roe Solver into CFL3D

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1 Roe-solver for Real Gas

The real-gas Roe solver is the one developed by Liou et. al [1], which was chosen in terms of its solid theoretical basis among other methods. In any case, Roe solver is derived from the Jacobian matrix,

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ \Pi_\rho - u^2 & 2u - u\Pi_{m_x} & \Pi_{m_y} & \Pi_{m_z} & \Pi_{E_s} \\ -uv & v & u & 0 & 0 \\ -uw & w & 0 & u & 0 \\ u(\Pi_\rho - H) & H + u\Pi_{m_x} & u\Pi_{m_y} & u\Pi_{m_z} & u(1+\Pi_{E_s}) \end{bmatrix} \tag{1}$$

for the 3D Euler equations

$$\mathbf{U}_t + \mathbf{A}\mathbf{U}_x + \mathbf{B}\mathbf{U}_y + \mathbf{C}\mathbf{U}_z = 0 \tag{2}$$

where $\mathbf{A} = \partial\mathbf{F}/\partial\mathbf{U}$,

$$\mathbf{U} = \begin{bmatrix} \rho \\ m_x \\ m_y \\ m_z \\ E_s \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ \rho uH \end{bmatrix}, \quad p = \Pi(\mathbf{U}), \quad H = [E_s + \Pi(\mathbf{U})]/\rho. \tag{3}$$

Note that all the complication comes from the pressure function $\Pi(\mathbf{U})$, i.e. a general EOS. The task is now to find the average state $\hat{\mathbf{U}}$ that satisfies $\Delta\mathbf{F} = \mathbf{A}\Delta\hat{\mathbf{U}}$ exactly. Straightforward calculation gives the usual Roe-average for u, v, w, and H as in the perfect-gas case, but one equation remains,

$$\Delta p = \hat{\Pi}_\rho \Delta\rho + \hat{\Pi}_{m_x}\Delta m_x + \hat{\Pi}_{m_y}\Delta m_y + \hat{\Pi}_{m_z}\Delta m_z + \hat{\Pi}_{E_s}\Delta E_s. \tag{4}$$

It is how to handle this relation that differentiates various real-gas extension of Roe's solver. In [1], Liou et. al set $p = p(e,\rho)$, and introduce additional Roe-averaged values $\hat{e}$ and $\hat{\rho}$ so that (4) becomes

$$\Delta p = \hat{p}_e \Delta e + \hat{p}_\rho \Delta\rho \tag{5}$$

where $\hat{p}_e$ and $\hat{p}_\rho$ are partial derivatives that remain to be defined. Note that $\bar{p}_e = p_e(\hat{e}, \hat{\rho})$ and $\bar{p}_\rho = p_\rho(\hat{e}, \hat{\rho})$ are easily computed by some difference formula but do not satisfy (5). To define the correct average derivatives, they regard (5) as a straight line in a plane of the two average derivatives (suitably scaled), and project the easily-computable values $\bar{p}_e$ and $\bar{p}_\rho$ onto that line to define $\hat{p}_e$ and $\hat{p}_\rho$. This gives the formulas for them in terms of known averaged quantities.

Now we have all necessary average quantities $(\hat{\rho}, \hat{u}, \hat{v}, \hat{w}, \hat{H}, \hat{e}, \hat{p}_e, \hat{p}_\rho)$ to compute the dissipation term in the Roe flux function. It is implemented in the following form.

$$|\mathbf{A}_n|\Delta\mathbf{U} = \begin{bmatrix} \ell_1 \\ u\ell_1 - an_x\ell_2 + \delta_u \\ v\ell_1 - an_y\ell_2 + \delta_v \\ w\ell_1 - an_z\ell_2 + \delta_w \\ H\ell_1 - au_n\ell_2 + u\delta_u + v\rho|u_n|\delta_v + w\delta_w - \frac{\rho a^2}{p_e}\alpha_2 \end{bmatrix} \tag{6}$$

where

$$\ell_1 = \alpha_1 + \alpha_2 + \alpha_5 \tag{7}$$
$$\ell_2 = \alpha_1 - \alpha_5 \tag{8}$$
$$\delta_u = \rho|u_n|(\Delta u - n_x\Delta u_n) \tag{9}$$
$$\delta_v = \rho|u_n|(\Delta v - n_y\Delta u_n) \tag{10}$$
$$\delta_w = \rho|u_n|(\Delta w - n_z\Delta u_n) \tag{11}$$
$$\alpha_1 = |u_n - a|\left(-\frac{\rho}{2a}\Delta u_n + \frac{\phi}{2}\right) \tag{12}$$
$$\alpha_2 = |u_n|\left(\Delta\rho - \phi\right) \tag{13}$$
$$\alpha_5 = |u_n + a|\left(\frac{\rho}{2a}\Delta u_n + \frac{\phi}{2}\right) \tag{14}$$
$$\phi = \frac{1}{H - V_s^2/2}\left[\Delta E_s - \left(\frac{V_s^2}{2}\Delta\rho + \rho\Delta(q^2/2)\right)\right] \tag{15}$$
$$\frac{V_s^2}{2} = H - \frac{\rho a^2}{p_e}. \tag{16}$$

It should be understood that all quantities in the above expressions are evaluated at the state $(\hat{\rho}, \hat{u}, \hat{v}, \hat{w}, \hat{H}, \hat{e}, \hat{p}_e, \hat{p}_\rho)$. The average speed of sound is given by

$$\hat{a} = \sqrt{\hat{p}_\rho + \hat{p}_e(\hat{H} - \hat{e} + \hat{q}^2/2)/\hat{\rho}} \tag{17}$$

For ideal gas, $\frac{\rho a^2}{p_e} = \frac{a^2}{\gamma - 1}$ and the solver reduces the Roe solver for ideal gas.

In order to implement this, we need subroutines for EOS that functions as $p = p(e, \rho)$. This is sufficient if there is no need to compute the energy for given pressure. In CFL3D, the variables it stores are primitive variables, and therefore we often need to compute energy from pressure. This requires a subroutine such as $e = e(p, \rho)$.

References

[1] M.-S. Liou, B van Leer, and J.-S. Shuen, JCP, **87**, 276, 1990.

