Species Decoupled Costate Variable Relationship Derivation

The purpose of this is to show the relationship between the costate variable for total density λ_ρ to the costate variables for species densities λ_{ρ_s}. Beginning with the definition of the Adjoint Equations:

$$\left(\frac{\partial R}{\partial Q}\right)^T \lambda = \frac{\partial F}{\partial Q} \tag{1}$$

Where the R is the residual of the governing equations, Q is the vector of conserved variables, and F is the cost function (i.e. lift, drag, etc.). Note that the first term is simply the transpose of the jacobian multiplied by the costate variable vector λ, and can be written as:

$$\left(\frac{\partial R}{\partial Q}\right)^T_i \lambda = \sum_{j=1}^{N_{eq}} \left(\frac{\partial R_j}{\partial Q_i}\right) \lambda_j \tag{2}$$

Suppose we define the system of equations in two different ways. The first system, which we'll call the "meanflow system", consists of 5 equations:

$$R = \begin{pmatrix} R_\rho \\ R_{\rho u} \\ R_{\rho v} \\ R_{\rho w} \\ R_{\rho E} \end{pmatrix}, \quad \lambda = \begin{pmatrix} \lambda_\rho \\ \lambda_{\rho u} \\ \lambda_{\rho v} \\ \lambda_{\rho w} \\ \lambda_{\rho E} \end{pmatrix} \tag{3}$$

The second system consists of the full system of equations:

$$R = \begin{pmatrix} R_{\rho_1} \\ \vdots \\ R_{\rho_s} \\ R_{\rho u} \\ R_{\rho v} \\ R_{\rho w} \\ R_{\rho E} \end{pmatrix}, \quad \lambda = \begin{pmatrix} \lambda_{\rho_1} \\ \vdots \\ \lambda_{\rho_s} \\ \lambda_{\rho u} \\ \lambda_{\rho v} \\ \lambda_{\rho w} \\ \lambda_{\rho E} \end{pmatrix} \tag{4}$$

By making the approximation that the mass fraction c_s is constant, we can show that the full system of equations reduces to the meanflow system. By this approximation the derivatives with respect to species density become:

$$\frac{\partial R}{\partial \rho} = \frac{\partial R}{\partial \rho_s}\frac{\partial \rho_s}{\partial \rho} = c_s \left(\frac{\partial R}{\partial \rho_s}\right) \tag{5}$$

Thus, for a single row of the full system:

$$\left(\frac{\partial R}{\partial Q}\right)^T_{\rho_s} \lambda = \sum_{j=1}^{N_{full}} \left(\frac{\partial R_j}{\partial \rho}\right) \frac{\lambda_j}{c_s} = \frac{1}{c_s}\left(\frac{\partial F}{\partial \rho}\right) \tag{6}$$

After cancelling the mass fractions, this allows the first row of the full system to be equated to the first row of the meanflow system:

$$\sum_{j=1}^{N_{full}} \left(\frac{\partial R_j}{\partial \rho}\right) \lambda_j = \sum_{j=1}^{N_{meanflow}} \left(\frac{\partial R_j}{\partial \rho}\right) \lambda_j \tag{7}$$

Expanding this out, it becomes clear many terms cancel:

$$\begin{aligned} &\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} + \frac{\partial R_{\rho u}}{\partial \rho}\lambda_{\rho u} + \frac{\partial R_{\rho v}}{\partial \rho}\lambda_{\rho v} + \frac{\partial R_{\rho w}}{\partial \rho}\lambda_{\rho w} + \frac{\partial R_{\rho E}}{\partial \rho}\lambda_{\rho E} = \\ &\qquad \frac{\partial R_{\rho}}{\partial \rho}\lambda_{\rho} + \frac{\partial R_{\rho u}}{\partial \rho}\lambda_{\rho u} + \frac{\partial R_{\rho v}}{\partial \rho}\lambda_{\rho v} + \frac{\partial R_{\rho w}}{\partial \rho}\lambda_{\rho w} + \frac{\partial R_{\rho E}}{\partial \rho}\lambda_{\rho E} \end{aligned} \tag{8}$$

$$\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} = \frac{\partial R_{\rho}}{\partial \rho}\lambda_{\rho} \tag{9}$$

Finally, because the individual species mass fluxes must sum to the total mass flux:

$$\sum_{s=1}^{N_{species}} R_{\rho_s} = R_{\rho} \tag{10}$$

Eqn (9) can be rewritten as:

$$\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} = \frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho} \tag{11}$$

Which implies that the species mass costate variables are all equal to the total mass costate variable, yielding:

$$\lambda_{\rho} = \lambda_{\rho_s} \tag{12}$$

$$d\lambda_{\rho} = d\lambda_{\rho_s} \tag{13}$$