Notes Towards PhD

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January 25, 2016

1 Adjoint Derivation

The FUN3D adjoint derivation is given in Eric Nielson's PhD Thesis. Starting with forming the Lagrangian as

$$L(\mathbf{D}, \mathbf{Q}, \mathbf{X}, \mathbf{\Lambda}) = f(\mathbf{D}, \mathbf{Q}, \mathbf{X}) + \mathbf{\Lambda}^T \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X}) \tag{1}$$

Where $\mathbf{R}$ is the residual of the flow equations. Differentiating with respect to the design variables $\mathbf{D}$ yields:

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{ \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}} \right\} + \left[\frac{\partial \mathbf{Q}}{\partial \mathbf{D}}\right]^T \left\{ \frac{\partial f}{\partial \mathbf{Q}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} \right\} + \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \right\} \mathbf{\Lambda} \tag{2}$$

To eliminate the dependence of conserved variables $\mathbf{Q}$ on the design variables, we solve the adjoint equation:

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} = -\frac{\partial f}{\partial \mathbf{Q}} \tag{3}$$

Where the Lagrange multipliers (also known as costate variables), $\mathbf{\Lambda}$ are the cost function dependence on the residual:

$$\mathbf{\Lambda} = -\frac{\partial f}{\partial \mathbf{R}} \tag{4}$$

This can ultimately be used to error estimation and sensitivity analysis for design optimization. With the second term in eq. (2) eliminated, the derivative of the Lagrangian becomes

$$\frac{\partial L}{\partial \mathbf{D}} = \left\{ \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \frac{\partial f}{\partial \mathbf{X}} \right\} + \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \right\} \mathbf{\Lambda} \tag{5}$$

By solving the adjoint equation in eq. (3) to obtain the costate variable vector, $\mathbf{\Lambda}$, we can now use a non-linear optimizer to determine the optimum set of design variables, $\mathbf{D}^*$. This can be done using **PORT** or **KSOPT** in FUN3D, as well as a host of other non-linear optimizers.

2 Decoupled Adjoint

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:

$$\left(\frac{\partial R}{\partial Q}\right)^T \lambda = \frac{\partial F}{\partial Q} \tag{6}$$

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:

$$\left(\frac{\partial R}{\partial Q}\right)_i^T \lambda = \sum_{j=1}^{N_{eq}} \left(\frac{\partial R_j}{\partial Q_i}\right) \lambda_j \tag{7}$$

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:

$$R = \begin{pmatrix} R_\rho \\ R_{\rho u} \\ R_{\rho v} \\ R_{\rho w} \\ R_{\rho E} \end{pmatrix}, \quad \lambda = \begin{pmatrix} \lambda_\rho \\ \lambda_{\rho u} \\ \lambda_{\rho v} \\ \lambda_{\rho w} \\ \lambda_{\rho E} \end{pmatrix} \tag{8}$$

The second system consists of the full system of equations:

$$R = \begin{pmatrix} R_{\rho_1} \\ \vdots \\ R_{\rho_s} \\ R_{\rho u} \\ R_{\rho v} \\ R_{\rho w} \\ R_{\rho E} \end{pmatrix}, \quad \lambda = \begin{pmatrix} \lambda_{\rho_1} \\ \vdots \\ \lambda_{\rho_s} \\ \lambda_{\rho u} \\ \lambda_{\rho v} \\ \lambda_{\rho w} \\ \lambda_{\rho E} \end{pmatrix} \tag{9}$$

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:

$$\frac{\partial R}{\partial \rho} = \frac{\partial R}{\partial \rho_s}\frac{\partial \rho_s}{\partial \rho} = c_s \left(\frac{\partial R}{\partial \rho_s}\right) \tag{10}$$

Thus, for a single row of the full system:

$$\left(\frac{\partial R}{\partial Q}\right)_{\rho_s}^T \lambda = \sum_{j=1}^{N_{full}} \left(\frac{\partial R_j}{\partial \rho}\right) \frac{\lambda_j}{c_s} = \frac{1}{c_s}\left(\frac{\partial F}{\partial \rho}\right) \tag{11}$$

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:

$$\sum_{j=1}^{N_{full}} \left(\frac{\partial R_j}{\partial \rho}\right) \lambda_j = \sum_{j=1}^{N_{meanflow}} \left(\frac{\partial R_j}{\partial \rho}\right) \lambda_j \tag{12}$$

Expanding this out, it becomes clear many terms cancel:

$$\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} + \frac{\partial R_{\rho u}}{\partial \rho}\lambda_{\rho u} + \frac{\partial R_{\rho v}}{\partial \rho}\lambda_{\rho v} + \frac{\partial R_{\rho w}}{\partial \rho}\lambda_{\rho w} + \frac{\partial R_{\rho E}}{\partial \rho}\lambda_{\rho E} =$$
$$\frac{\partial R_{\rho}}{\partial \rho}\lambda_{\rho} + \frac{\partial R_{\rho u}}{\partial \rho}\lambda_{\rho u} + \frac{\partial R_{\rho v}}{\partial \rho}\lambda_{\rho v} + \frac{\partial R_{\rho w}}{\partial \rho}\lambda_{\rho w} + \frac{\partial R_{\rho E}}{\partial \rho}\lambda_{\rho E} \quad (13)$$

$$\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} = \frac{\partial R_{\rho}}{\partial \rho}\lambda_{\rho} \quad (14)$$

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

$$\sum_{s=1}^{N_{species}} R_{\rho_s} = R_{\rho} \quad (15)$$

Eqn (14) can be rewritten as:

$$\frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho_1} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho_s} = \frac{\partial R_{\rho_1}}{\partial \rho}\lambda_{\rho} + \cdots + \frac{\partial R_{\rho_s}}{\partial \rho}\lambda_{\rho} \quad (16)$$

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

$$\lambda_{\rho} = \lambda_{\rho_s} \quad (17)$$
$$d\lambda_{\rho} = d\lambda_{\rho_s} \quad (18)$$

A. Decoupled Flux Derivation

For the Roe Flux Difference Splitting scheme, the species mass fluxes are given by:

$$F_{\rho_s} = \frac{\rho_s^L \overline{U}^L + \rho_s^R \overline{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_{3_s})}{2} \tag{19}$$

$$dv_1 = \frac{p^R - p^L + \tilde{\rho}\tilde{a}(\overline{U}^R - \overline{U}^L)}{\tilde{a}^2} \tag{20}$$

$$dv_2 = \frac{p^R - p^L - \tilde{\rho}\tilde{a}(\overline{U}^R - \overline{U}^L)}{\tilde{a}^2} \tag{21}$$

$$dv_{3_s} = \frac{\tilde{a}^2(\rho_s^R - \rho_s^L) - \tilde{c}_s(p^R - p^L)}{\tilde{a}^2} \tag{22}$$

$$\lambda_1 = \mid \overline{\mathbf{U}} + \tilde{a} \mid, \quad \lambda_2 = \mid \overline{\mathbf{U}} - \tilde{a} \mid, \quad \lambda_3 = \mid \overline{\mathbf{U}} \mid \tag{23}$$

where the ˜ notation signifies a roe-averaged quantity, given by:

$$\tilde{\mathbf{U}} = w\tilde{\mathbf{U}}^L + (1-w)\tilde{\mathbf{U}}^R \tag{24}$$

$$w = \frac{\tilde{\rho}}{\tilde{\rho} + \rho^R} \tag{25}$$

The species mass fluxes must sum to the total mass flux; thus, the total mixture mass flux is given as:

$$F_\rho = \sum_s F_{\rho_s} = \frac{\rho^L \overline{U}^L + \rho^R \overline{U}^R}{2} - \frac{\tilde{c}_s(\lambda_1 dv_1 + \lambda_2 dv_2) + \lambda_3 dv_3)}{2} \tag{26}$$

$$dv_3 = \frac{\tilde{a}^2(\rho^R - \rho^L) - (p^R - p^L)}{\tilde{a}^2} \tag{27}$$

Multiplying eq. (26) by the roe-averaged mass fraction and substituting into eq. (19) results in:

$$F_{\rho_s} = \tilde{c}_s F_\rho + \frac{(c_s^L - \tilde{c}_s)\rho^L(\overline{U}^L + \mid \tilde{U} \mid)}{2} + \frac{(c_s^R - \tilde{c}_s)\rho^R(\overline{U}^R - \mid \tilde{U} \mid)}{2} \tag{28}$$

The notation can be further simplified by defining the normal velocities as follows:

$$\lambda^+ = \frac{\overline{U}^L + \mid \tilde{U} \mid}{2}, \quad \lambda^- = \frac{\overline{U}^R - \mid \tilde{U} \mid}{2} \tag{29}$$

Finally, substituting Eq. (29) into Eq. (28) yields the final result for calculating the species flux in the decoupled system:

$$F_{\rho_s} = \tilde{c}_s F_\rho + (c_s^L - \tilde{c}_s)\rho^L \lambda^+ + (c_s^R - \tilde{c}_s)\rho^R \lambda^- \tag{30}$$

Forming the convective contributions to the Jacobians is straightforward. Because the $\mathbf{U}'$ level variables are constant, only the left, right, and roe-averaged state mass fractions vary. Differentiating Eq. (30) with respect to the mass fraction, c_s, the left and right state contributions are:

$$\frac{\partial F_{\rho_s}}{\partial c_s^L} = wF_\rho + (1-w)\rho^L\lambda^+ - w\rho^R\lambda^- \tag{31}$$

$$\frac{\partial F_{\rho_s}}{\partial c_s^R} = (1-w)F_\rho + (w-1)\rho^L\lambda^+ + w\rho^R\lambda^- \tag{32}$$

Because there is no dependence between species in decoupled convective formulation, the Jacobian block elements are purely diagonal for the convective contributions, of the form:

$$\begin{pmatrix} \frac{\partial F_{\rho_1}}{\partial c_1} & & 0 \\ & \ddots & \\ 0 & & \frac{\partial F_{\rho_{ns}}}{\partial c_{ns}} \end{pmatrix} \tag{33}$$

3 Thrust Optimization

A simple optimization example for an hypersonic testcase is to determine a level of thrust for a Supersonic Retro-Propulsion (SRP) blunt body geometry. The grid used for this test is a structured grid, show in figure 1 The nozzle parameters has a number of degrees of freedom with regard to

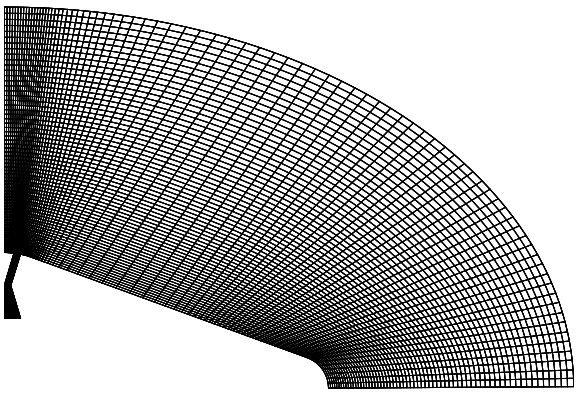

Figure 1: SRP Configuration Grid

user input. Combustion products can be specified separately from the freestream flow, and will be mixed in as the solution progresses in time. Additionally, the total pressure and temperature in the nozzle plenum can be specified. Through testing, this particular configuration has been determined to be steady and is therefore a good candidate for testing with the adjoint. In terms of optimization, this case can be optimized for maximum drag, using a number of design parameters.

The simplist design parameter is total pressure and/or temperature in the nozzle plenum. This results in a significant simplification of the objective function to be minimized, because there is no mesh dependence on the design variables; thus, eq. (5) can be simplified to

$$\frac{\partial L}{\partial \mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \frac{\partial \mathbf{R}}{\partial \mathbf{D}}^T \mathbf{\Lambda} \tag{34}$$

Now the cost function and residual dependence upon the plenum initial conditions must be derived. For the drag cost function, this is achieved by looping over all of the surface faces and linearizing the drag cost function w.r.t. the pressure/temperature (CHECK THIS!). For the residual, the

4 Specific Heat Derivatives

NOTE: THIS IS NOT USED (we're linearly interpolating)

In order to check Specific heat (C_p) derivatives from the curve fits, C_p and species enthalpy (h_{ij}) must have continuous derivatives. This is not inherently the case from the Gordon-McBride curve fits employed; therefore blending is employed to ensure that both C_p and h_{ij} are C_1 and C_0 continuous. The blending is implemented as

$$C_p = f_n C_{p_n} + f_m C_{p_m} \tag{35}$$

$$h_{ij} = \int C_p dT = \int (f_n C_{p_n} + f_m C_{p_m}) dT \tag{36}$$

The curve fits defined by Gordon-McBride are a 7th-degree polynomial of the form

$$C_p = \sum_{i=1}^{7} C_i T^{i-3} \tag{37}$$

And the blending parameters, f_n and f_m are

$$f_n = \begin{cases} \frac{1}{2dT_h}(T_u - T) & (T_u - dT_h) < T \leq T_u \\ \frac{1}{2dT_l}(T - T_l) & T_l < T \leq (T_l + dT_h) \end{cases} \tag{38}$$

$$dT_h = \frac{T_u}{100} \quad dT_l = \frac{T_l}{100} \tag{39}$$

$$f_m = 1 - f_n \tag{40}$$

Where T_u and T_l are the upper and lower valid temperature bounds on a range. Thus, substituting into eqn. (36) yields

$$h_{ij} = \int \left(f_n \sum_{i=1}^{7} C_{n_i} T^{i-3} + (1 - f_n) \sum_{i=1}^{7} C_{m_i} T^{i-3} \right) dT \tag{41}$$

If $(T_u - dT_h) < T \leq T_u$, integrating eqn. (41) yields

$$h_{ij} = 50h_n - \frac{50}{T_u} \left(C_{n_1} \ln(T) + \sum_{i=2}^{7} \frac{C_{n_i} T^{i-1}}{i-1} \right) - 49h_m + \frac{50}{T_u} \left(C_{m_1} \ln(T) + \sum_{i=2}^{7} \frac{C_{m_i} T^{i-1}}{i-1} \right) + C \tag{42}$$

Where

$$h_n = \int C_{p_n} dT, \quad h_m = \int C_{p_m} dT \tag{43}$$

If $T_l < T \leq (T_l + dT_h)$, integrating eqn. (41) yields

$$h_{ij} = -50h_n + \frac{50}{T_l}\left(C_{n_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{n_i}T^{i-1}}{i-1}\right) + 49h_m - \frac{50}{T_l}\left(C_{m_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{m_i}T^{i-1}}{i-1}\right) + C \tag{44}$$

It quickly becomes apparent that eqn.s (42) and (44) can be combined into

$$h_{ij} = \lambda\left[50h_n - \frac{2}{dT_s}\left(C_{n_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{n_i}T^{i-1}}{i-1}\right) - 49h_m + \frac{2}{dT_s}\left(C_{m_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{m_i}T^{i-1}}{i-1}\right)\right] + C \tag{45}$$

with

$$\lambda,\ dT_s = \begin{cases} 1,\ dT_u & (T_u - dT_h) < T \leq T_u \\ -1,\ dT_l & T_l < T \leq (T_l + dT_h) \end{cases} \tag{46}$$

To detemine the constant of integration, C, we use the condition

$$h_{ij}(T_{co}) = \frac{1}{2}(h_n(T_{co}) + h_m(T_{co})), \quad T_{co} = T_u = T_l \tag{47}$$

which specifies that the enthalpy at the intersection of temperature ranges should the average of the enthalpy in the respective ranges. Evaluating eqn. (45) with condition provided my eqn. (47) yields

$$\begin{aligned} C = {} & (\frac{1}{2} - 50\lambda)h_n\ |_{T=T_{co}}) + (\frac{1}{2} + 49\lambda)h_m\ |_{T=T_{co}}) \\ & + \frac{2\lambda}{dT_s}(C_{n_1}\ln(T_{co}) + \sum_{i=2}^{7}\frac{C_{n_i}T_{co}^{i-1}}{i-1}) \\ & - \frac{2\lambda}{dT_s}(C_{m_1}\ln(T_{co}) + \sum_{i=2}^{7}\frac{C_{m_i}T_{co}^{i-1}}{i-1}) \end{aligned} \tag{48}$$

Inserting into eq. (48), the final form of the blended enthalpy function is

$$\begin{aligned} h_{ij} = {} & \lambda\left[50h_n - \frac{2}{dT_s}\left(C_{n_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{n_i}T^{i-1}}{i-1}\right) - 49h_m + \frac{2}{dT_s}\left(C_{m_1}\ln(T) + \sum_{i=2}^{7}\frac{C_{m_i}T^{i-1}}{i-1}\right)\right] \\ & + (\frac{1}{2} - 50\lambda)h_n\ |_{T=T_{co}}) + (\frac{1}{2} + 49\lambda)h_m\ |_{T=T_{co}}) \\ & + \frac{2\lambda}{dT_s}\left(C_{n_1}\ln(T_{co}) + \sum_{i=2}^{7}\frac{C_{n_i}T_{co}^{i-1}}{i-1}\right) \\ & - \frac{2\lambda}{dT_s}\left(C_{m_1}\ln(T_{co}) + \sum_{i=2}^{7}\frac{C_{m_i}T_{co}^{i-1}}{i-1}\right) \end{aligned} \tag{49}$$