Decoupled adjoint formulation

Kyle B. Thompson

October 21, 2016

The primal flow equations are solved using the decoupled scheme based on the work by Candler, et. al. In doing this the conserved variables are split from

$$\mathbf{U} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix} \tag{1}$$

into

$$\mathbf{U}' = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{pmatrix}, \qquad \hat{\mathbf{U}} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \end{pmatrix} \tag{2}$$

By doing this, the flow equations can be solved implicitly using an approximate, first-order jacobian to drive the flow solution to a converged steady-state. In practice, this is done by essentially formulating

$$\frac{V}{\Delta t}\mathbf{I} + \begin{pmatrix} \frac{\partial \mathbf{R}_\rho}{\partial \rho} & \frac{\partial \mathbf{R}_\rho}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_\rho}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix} \begin{pmatrix} \Delta \rho \\ \Delta \rho \mathbf{u} \\ \Delta \rho E \end{pmatrix} = \begin{pmatrix} \mathbf{R}_\rho \\ \mathbf{R}_{\rho \mathbf{u}} \\ \mathbf{R}_{\rho E} \end{pmatrix} \tag{3}$$

to solve for the mixture flow variables, and formulating

$$\frac{V}{\Delta t}\mathbf{I} + \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial c_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_1}}{\partial c_{ns}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial c_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial c_{ns}} \end{pmatrix} \begin{pmatrix} \Delta c_1 \\ \vdots \\ \Delta c_{ns} \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{\rho_1} \\ \vdots \\ \mathbf{R}_{\rho_{ns}} \end{pmatrix} \tag{4}$$

Note that the correction terms required to maintain $\sum_{s=1}^{ns} c_s = 1$ and $\sum_{s=1}^{ns} \delta c_s = 0$ are omitted in Eq. (4) only for brevity in this explanation. Examining Eq.s (3-4) shows that there are clearly some physical dependencies being omitted, namely $\frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}$, $\frac{\partial \mathbf{R}_{\rho}}{\partial c_s}$, $\frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial c_s}$, and $\frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}$. It has been demonstrated that omitting this dependencies does not hinder convergence the primal solver; however, the adjoint requires an exact linearization of the converged steady-state solution.

The discrete adjoint formulation is given as

$$\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \mathbf{\Lambda} = -\frac{\partial f}{\partial \mathbf{Q}} \tag{5}$$

where $\mathbf{Q}$ is a vector of conserved variables, and f is the cost function (i.e. lift, drag, etc.). There is now an apparent need to reconcile the two sets of conserved variables in Eq. (2) with $\mathbf{Q}$. The most intuitive and staightforward way to do this is to forgo solving for the species mass ρ_s in lieu of the species mass fraction c_s. Thus, $\mathbf{Q}$ can be expressed as

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \\ c_1 \\ \vdots \\ c_{ns} \end{pmatrix} \tag{6}$$

This allows the linearizations derived in Eq.s (3-4) to be used in the adjoint formulation, by augmenting them with the previously omitted linearizations. Replacing $\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}$ with the fully system, the adjoint system becomes

$$\begin{pmatrix} \frac{\partial \mathbf{R}_{\rho}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho E}^T & \frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T \end{pmatrix} \begin{pmatrix} \Lambda_{\rho} \\ \Lambda_{\rho \mathbf{u}} \\ \Lambda_{\rho E} \\ \Lambda_{c_s} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho} \\ \frac{\partial f}{\partial \rho \mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \\ \frac{\partial f}{\partial c_s} \end{pmatrix} \tag{7}$$

Thus the jacobian in Eq. (7) is the completed one of Eq.s (3-4). While this is useful, the point of decoupling the species equations from the mixture equations was to speed up the linear solver and save memory. Solving Eq. (7) undermines both of these goals, so an alternative solution strategy must be formulated. If a block jacobi scheme is employed, the system can be decoupled once again as

$$\begin{pmatrix} \frac{\partial \mathbf{R}_{\rho}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T \end{pmatrix} \begin{pmatrix} \Lambda_{\rho} \\ \Lambda_{\rho \mathbf{u}} \\ \Lambda_{\rho E} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho} \\ \frac{\partial f}{\partial \rho \mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \end{pmatrix} - \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T \end{pmatrix} \Lambda_{c_s} \tag{8}$$

$$\frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T \Lambda_{c_s} = -\frac{\partial f}{\partial c_s} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}^T \Lambda_{\rho} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho \mathbf{u}}^T \Lambda_{\rho \mathbf{u}} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho E}^T \Lambda_{\rho E} \tag{9}$$

If a time-like derivative is added to the adjoint, the solution of the costate variables, Λ, can be time marched similar to the primal flow solver

$$\left[\frac{V}{\Delta t}\mathbf{I} + \frac{\partial \mathbf{R}}{\partial \mathbf{Q}}^T\right]\Delta\Lambda = -\frac{\partial f}{\partial \mathbf{Q}} - \frac{\partial \mathbf{R}}{\partial \mathbf{Q}}^T\Lambda \tag{10}$$

Thus, the first system in Eq. (8) becomes

$$\begin{aligned}\left[\frac{V}{\Delta t}\mathbf{I} + \begin{pmatrix} \frac{\partial \mathbf{R}_\rho}{\partial \rho}^T & \frac{\partial \mathbf{R}_\rho}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_\rho}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T \end{pmatrix}\right]\begin{pmatrix}\Delta\Lambda_\rho \\ \Delta\Lambda_{\rho\mathbf{u}} \\ \Delta\Lambda_{\rho E}\end{pmatrix} = \\ -\begin{pmatrix}\frac{\partial f}{\partial \rho} \\ \frac{\partial f}{\partial \rho\mathbf{u}} \\ \frac{\partial f}{\partial \rho E}\end{pmatrix} - \begin{pmatrix} \frac{\partial \mathbf{R}_\rho}{\partial \rho}^T & \frac{\partial \mathbf{R}_\rho}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_\rho}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}^T & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}^T \end{pmatrix}\begin{pmatrix}\Lambda_\rho \\ \Lambda_{\rho\mathbf{u}} \\ \Lambda_{\rho E}\end{pmatrix} - \begin{pmatrix}\frac{\partial \mathbf{R}_\rho}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial c_s}^T \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}^T\end{pmatrix}\Lambda_{c_s}\end{aligned} \tag{11}$$

and the second system in Eq. (9) becomes

$$\left(\frac{V}{\Delta t}\mathbf{I} + \frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T\right)\Delta\Lambda_{c_s} = -\frac{\partial f}{\partial c_s} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial c_s}^T\Lambda_{c_s} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho}^T\Lambda_\rho - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho\mathbf{u}}^T\Lambda_{\rho\mathbf{u}} - \frac{\partial \mathbf{R}_{\rho_s}}{\partial \rho E}^T\Lambda_{\rho E} \tag{12}$$

This is advantageous, because the jacobians on the left hand side (LHS) can be the first-order approximate jacobians that were used to solve the primal flow equations; hence, all of the benefits of the diagonal block matricies that are exploited to reduce the linear solver cost and overall memory now apply to the adjoint.