Change of Variables

Kyle B. Thompson

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0.1 Change of Variable Sets

The decoupled scheme developed by Candler et. al is based upon the change of variables

$$\mathbf{U} = \begin{pmatrix} \rho_1 \\ \vdots \\ \rho_{ns} \\ \rho\mathbf{u} \\ \rho E \end{pmatrix} \rightarrow \mathbf{V} = \begin{pmatrix} c_1 \\ \vdots \\ c_{ns} \\ \rho \\ \rho\mathbf{u} \\ \rho E \end{pmatrix} \tag{1}$$

To avoid confusion between variable sets, we re-write the variable vectors, $\mathbf{U}$ and $\mathbf{V}$, in a more generic sense

$$\mathbf{U} = \begin{pmatrix} u_1 \\ \vdots \\ u_{ns+2} \end{pmatrix} \rightarrow \mathbf{V} = \begin{pmatrix} v_1 \\ \vdots \\ v_{ns+3} \end{pmatrix} \tag{2}$$

For simplicity, consider a system with two species, ρ_1 and ρ_2. Using the relationship $\rho_s = c_s \rho$, then the original variable vector, $\mathbf{U}$ can be rewritten in terms of the new variables, $\mathbf{V}$ as

$$\mathbf{U} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} v_1 v_3 \\ v_2 v_3 \\ v_4 \\ v_5 \end{pmatrix} \tag{3}$$

This allows the derivation of the jacobian

$$\frac{\partial \mathbf{U}}{\partial \mathbf{V}} = \begin{pmatrix} \frac{\partial u_1}{\partial v_1} & \frac{\partial u_1}{\partial v_2} & \frac{\partial u_1}{\partial v_3} & \frac{\partial u_1}{\partial v_4} & \frac{\partial u_1}{\partial v_5} \\ \frac{\partial u_2}{\partial v_1} & \frac{\partial u_2}{\partial v_2} & \frac{\partial u_2}{\partial v_3} & \frac{\partial u_2}{\partial v_4} & \frac{\partial u_2}{\partial v_5} \\ \frac{\partial u_3}{\partial v_1} & \frac{\partial u_3}{\partial v_2} & \frac{\partial u_3}{\partial v_3} & \frac{\partial u_3}{\partial v_4} & \frac{\partial u_3}{\partial v_5} \\ \frac{\partial u_4}{\partial v_1} & \frac{\partial u_4}{\partial v_2} & \frac{\partial u_4}{\partial v_3} & \frac{\partial u_4}{\partial v_4} & \frac{\partial u_4}{\partial v_5} \end{pmatrix} = \begin{pmatrix} v_3 & 0 & v_1 & 0 & 0 \\ 0 & v_3 & v_2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{4}$$

At this point, it is important to note that the jacobian in Eq. (4) has two psuedo-inverse matricies, that correspond to the right and left inverse. The right inverse, $\frac{\partial \mathbf{V}}{\partial \mathbf{U}}\Big|_R$, can be constructed based on the previously defined steps

$$\frac{\partial \mathbf{V}}{\partial \mathbf{U}}\Big|_R = \begin{pmatrix} \frac{\partial v_1}{\partial u_1} & \frac{\partial v_1}{\partial u_2} & \frac{\partial v_1}{\partial u_3} & \frac{\partial v_1}{\partial u_4} \\ \frac{\partial v_2}{\partial u_1} & \frac{\partial v_2}{\partial u_2} & \frac{\partial v_2}{\partial u_3} & \frac{\partial v_2}{\partial u_4} \\ \frac{\partial v_3}{\partial u_1} & \frac{\partial v_3}{\partial u_2} & \frac{\partial v_3}{\partial u_3} & \frac{\partial v_3}{\partial u_4} \\ \frac{\partial v_4}{\partial u_1} & \frac{\partial v_4}{\partial u_2} & \frac{\partial v_4}{\partial u_3} & \frac{\partial v_4}{\partial u_4} \\ \frac{\partial v_5}{\partial u_1} & \frac{\partial v_5}{\partial u_2} & \frac{\partial v_5}{\partial u_3} & \frac{\partial v_5}{\partial u_4} \end{pmatrix} = \begin{pmatrix} \frac{1-v_1}{v_3} & \frac{-v_1}{v_3} & 0 & 0 \\ \frac{-v_2}{v_3} & \frac{1-v_2}{v_3} & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5}$$

It is easily verified that the matrix product of Eq.s (4-5) produces identity

$$\frac{\partial \mathbf{U}}{\partial \mathbf{V}} \left.\frac{\partial \mathbf{V}}{\partial \mathbf{U}}\right|_R = \begin{pmatrix} v_3 & 0 & v_1 & 0 & 0 \\ 0 & v_3 & v_2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1-v_1}{v_3} & \frac{-v_1}{v_3} & 0 & 0 \\ \frac{-v_2}{v_3} & \frac{1-v_2}{v_3} & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{6}$$

however, Eq. (6) is not associative

$$\begin{aligned} \left.\frac{\partial \mathbf{V}}{\partial \mathbf{U}}\right|_R \frac{\partial \mathbf{U}}{\partial \mathbf{V}} &= \begin{pmatrix} \frac{1-v_1}{v_3} & \frac{-v_1}{v_3} & 0 & 0 \\ \frac{-v_2}{v_3} & \frac{1-v_2}{v_3} & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_3 & 0 & v_1 & 0 & 0 \\ 0 & v_3 & v_2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1-v_1 & -v_1 & \frac{-(v_1)^2-v_1v_2+v_1}{v_3} & 0 & 0 \\ -v_2 & 1-v_2 & \frac{-(v_2)^2-v_1v_2+v_2}{v_3} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned} \tag{7}$$

to correctly compute identity, the property of matrix transpose multiplication is used

$$\left(\frac{\partial \mathbf{U}}{\partial \mathbf{V}} \frac{\partial \mathbf{V}}{\partial \mathbf{U}}\bigg|_R\right)^T = \frac{\partial \mathbf{V}}{\partial \mathbf{U}}\bigg|_R^T \frac{\partial \mathbf{U}}{\partial \mathbf{V}}^T$$
$$= \begin{pmatrix} \frac{1-v_1}{v_3} & \frac{-v_2}{v_3} & 1 & 0 & 0 \\ \frac{-v_1}{v_3} & \frac{1-v_2}{v_3} & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_3 & 0 & 0 & 0 \\ 0 & v_3 & 0 & 0 \\ v_1 & v_2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{8}$$
$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This is critical in understanding the relationships needed to switch transform variables sets. For linearizations of the residual, $\mathbf{R}$, the correct transformation from the variable set $\mathbf{U}$ to the variable set $\mathbf{V}$ is

$$\frac{\partial \mathbf{R}}{\partial \mathbf{V}} = \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial \mathbf{V}} \tag{9}$$

which is intuitively understood; however, the transformation from the variable set $\mathbf{V}$ to the variable set $\mathbf{U}$ must follow Eq. (8)

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}} = \left(\frac{\partial \mathbf{R}}{\partial \mathbf{V}}^T \frac{\partial \mathbf{V}}{\partial \mathbf{U}}^T\right)^T \tag{10}$$

The transposition in Eq. (9) is critical, as the linearizations will be incorrect if the multiplication is done without it. Fortunately, Eq. (9) is rarely seen in practice, as most linearizations are done for the fully-coupled system that requires Eq. (10) to transform the linearizations

$$\frac{\partial \mathbf{R}}{\partial \mathbf{V}} = \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \frac{\partial \mathbf{U}}{\partial \mathbf{V}} = \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1} & \dots & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_1} & \dots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1} & \dots & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1} & \dots & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix} \begin{pmatrix} \rho & \dots & 0 & c_1 & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \rho & c_{ns} & 0 & 0 \\ 0 & \dots & 0 & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 0 & 1 \end{pmatrix} \tag{11}$$

likewise, in the adjoint the transformation is applied to the tranpose of the jacobian

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T = \frac{\partial \mathbf{U}}{\partial \mathbf{V}}^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T = \begin{pmatrix} \rho & \dots & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & \rho & 0 & 0 \\ c_1 & \dots & c_{ns} & 0 & 0 \\ 0 & \dots & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1} & \dots & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho_1} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}} & \dots & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}} & \dots & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E} & \dots & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho E} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix} \tag{12}$$

Since the tranformation is right-multiplied, the matrix vector products of the exact jacobian with costate variables, Λ, in the adjoint linear system can be done first, and the transformation can then be applied to the system

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T \Lambda = \begin{pmatrix} \rho & \dots & 0 & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & \dots & \rho & 0 & 0 \\ c_1 & \dots & c_{ns} & 0 & 0 \\ 0 & \dots & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1}\Lambda_{\rho_1} & \dots & + & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho_1}\Lambda_{\rho_{ns}} & + & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1}\Lambda_{\rho \mathbf{u}} & + & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1}\Lambda_{\rho E} \\ \vdots & \ddots & & \vdots & & \vdots & & \vdots \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}}\Lambda_{\rho_1} & \dots & + & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho_{ns}}\Lambda_{\rho_{ns}} & + & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}}\Lambda_{\rho \mathbf{u}} & + & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}}\Lambda_{\rho E} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}}\Lambda_{\rho_1} & \dots & + & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho \mathbf{u}}\Lambda_{\rho_{ns}} & + & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}}\Lambda_{\rho \mathbf{u}} & + & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}}\Lambda_{\rho E} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E}\Lambda_{\rho_1} & \dots & + & \frac{\partial \mathbf{R}_{\rho ns}}{\partial \rho E}\Lambda_{\rho_{ns}} & + & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E}\Lambda_{\rho \mathbf{u}} & + & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}\Lambda_{\rho E} \end{pmatrix} \tag{13}$$

This indicates the important point that the transformation of the adjoint residual is not dependent on the number of equations solved, but only the number of dependent variables the equations are linearized with respect to, namely $\mathbf{U}$.

In the decoupled scheme the number of equations effectively solved is one more than the fully-coupled scheme. The residual vector, R for the decoupled scheme can be written as

$$\mathbf{R} = \begin{pmatrix} \mathbf{R}_{\rho_1} - c_1 \sum_{i=1}^{N_s} (\mathbf{R}_{\rho_i}) \\ \vdots \\ \mathbf{R}_{\rho_{N_s}} - c_{N_s} \sum_{i=1}^{N_s} (\mathbf{R}_{\rho_i}) \\ \sum_{i=1}^{N_s} (\mathbf{R}_{\rho_i}) \\ \mathbf{R}_{\rho \mathbf{u}} \\ \mathbf{R}_{\rho E} \end{pmatrix} \tag{14}$$

The residual vector in Eq. (14) is composed entirely of components from the fully coupled system;

there for the linearizations for the fully-coupled system can be re-used to construct the decoupled adjoint residual

0.2 Relationship to Adjoint Equation

The flow solver equations can be constructed by the integration of the governing equations. In semi-discrete form, this is

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{1}{V}\sum_{i}^{N_{nodes}} (\mathbf{F}_i \cdot \mathbf{n}_i) = \mathbf{W} \tag{15}$$

where

$$\mathbf{F} = \begin{pmatrix} \rho_1 \mathbf{u} \\ \vdots \\ \rho_{N_s} \\ \rho \mathbf{u}^2 + p\mathbf{n} \\ (E+p)\mathbf{u} \end{pmatrix} \tag{16}$$

the next time level $n+1$ can be determined from the current time level n if the equations are linearized by the approximations

$$\begin{aligned} \mathbf{F}^{n+1} &\approx \mathbf{F}^n + \frac{\partial \mathbf{F}^n}{\partial \mathbf{U}} d\mathbf{U}^n \\ \mathbf{W}^{n+1} &\approx \mathbf{W}^n + \frac{\partial \mathbf{W}^n}{\partial \mathbf{U}} d\mathbf{U}^n \end{aligned} \tag{17}$$

This creates the linear system of equations which may be solved by a quasi-Newton method

$$\left[\frac{V}{\Delta t}\mathbf{I} + \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix} \right] \begin{pmatrix} d\rho_1 \\ \vdots \\ d\rho_{N_s} \\ d\rho \mathbf{u} \\ d\rho E \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{\rho_1} \\ \vdots \\ \mathbf{R}_{\rho_{N_s}} \\ \mathbf{R}_{\rho \mathbf{u}} \\ \mathbf{R}_{\rho E} \end{pmatrix} \tag{18}$$

assuming all linearizations are exact, the adjoint system of equations that results from the fully coupled formulation in Eq. (18) is

$$\begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_1} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} \\ \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho E} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix} \begin{pmatrix} \Lambda_{\rho_1} \\ \vdots \\ \Lambda_{\rho_{N_s}} \\ \Lambda_{\rho \mathbf{u}} \\ \Lambda_{\rho E} \end{pmatrix} = - \begin{pmatrix} \frac{\partial f}{\partial \rho_1} \\ \vdots \\ \frac{\partial f}{\partial \rho_{N_s}} \\ \frac{\partial f}{\partial \rho \mathbf{u}} \\ \frac{\partial f}{\partial \rho E} \end{pmatrix} \tag{19}$$

In the new variable set, $\mathbf{V}$, Eq. (18) is re-written as

$$\left[\frac{V}{\Delta t}\mathbf{I} + \begin{pmatrix} \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_1}}{\partial \rho E} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho_{ns}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho \mathbf{u}}}{\partial \rho E} \\ \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_1} & \cdots & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho_{ns}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho \mathbf{u}} & \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E} \end{pmatrix}\right] \begin{pmatrix} dc_1 \\ \vdots \\ dc_{N_s} \\ d\rho \\ d\rho\mathbf{u} \\ d\rho E \end{pmatrix} = \begin{pmatrix} \mathbf{R}'_{\rho_1} \\ \vdots \\ \mathbf{R}'_{\rho_{N_s}} \\ \mathbf{R}_{\rho} \\ \mathbf{R}_{\rho\mathbf{u}} \\ \mathbf{R}_{\rho E} \end{pmatrix} \tag{20}$$

Where the new species density equations $\mathbf{R}'_{\rho_s}$ and mixture density equation $\mathbf{R}_\rho$ are defined as

$$\mathbf{R}'_{\rho_s} = \mathbf{R}_{\rho_s} - c_s \mathbf{R}_\rho \tag{21}$$

$$\mathbf{R}_\rho = \sum_{i=1}^{N_s} \left(\mathbf{R}_{\rho_i}\right) \tag{22}$$

Eq.s (21-22) are critical to the adjoint formulation of Eq. (20), as primal flow equations have been altered to enforce the constraint that

$$\sum_{i=1}^{N_s} (c_i) = 1, \quad \sum_{i=1}^{N_s} (dc_i) = 0, \tag{23}$$

Just as relationships were derived for the variables set $\mathbf{U}$ and $\mathbf{V}$ in Section 0.1, there are also relationships between the equations, which we denote as $\mathbf{R_U}$ and $\mathbf{R_V}$ for the variable sets $\mathbf{U}$ and $\mathbf{V}$, respectively. the equation set $\mathbf{R_U}$ can be rewritten in terms of the equation set $\mathbf{R_V}$, to form the jacobian

$$\mathbf{R_U} = \begin{pmatrix} \mathbf{R}_{\mathbf{V}_i} + c_i \left(\mathbf{R}_{\mathbf{V}_{N_s+1}}\right) \\ \mathbf{R}_{\mathbf{V}_{N_s+2}} \\ \mathbf{R}_{\mathbf{V}_{N_s+3}} \end{pmatrix} \tag{24}$$

$$\frac{\partial \mathbf{R_U}}{\partial \mathbf{R_V}} = \begin{pmatrix} 1 & 0 & c_i & 0 & 0 \\ 0 & 1 & c_i & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{25}$$

Likewise, the tranformation can be made from $\mathbf{R_V}$ to $\mathbf{R_U}$

$$\mathbf{R_V} = \begin{pmatrix} \mathbf{R_U}_i + c_i \sum_{k=1}^{N_s} (\mathbf{R_U}_k) \\ \\ \sum_{k=1}^{N_s} (\mathbf{R_U}_k) \\ \\ \mathbf{R_U}_{N_s+1} \\ \\ \mathbf{R_U}_{N_s+2} \end{pmatrix} \tag{26}$$

$$\frac{\partial \mathbf{R_V}}{\partial \mathbf{R_U}} = \begin{pmatrix} 1-c_i & -c_i & 0 & 0 \\ \\ -c_i & 1-c_i & 0 & 0 \\ \\ 1 & 1 & 0 & 0 \\ \\ 0 & 0 & 1 & 0 \\ \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{27}$$

The change of equations sets in Eq.s (24-25) and the change of dependent variable in Eq. (3) can be used to rewrite the fully coupled system in Eq. (18) into the decoupled system from Eq. (20)

$$\begin{gathered} \left(\frac{V}{\Delta t}\mathbf{I} + \frac{\partial \mathbf{R_U}}{\partial \mathbf{U}}\right) d\mathbf{U} = \mathbf{R_U} \\ \frac{\partial \mathbf{R_V}}{\partial \mathbf{R_U}} \left(\frac{V}{\Delta t}\mathbf{I} + \frac{\partial \mathbf{R_U}}{\partial \mathbf{U}}\right) \left(\frac{\partial \mathbf{U}}{\partial \mathbf{V}}\right) d\mathbf{V} = \frac{\partial \mathbf{R_V}}{\partial \mathbf{R_U}} \mathbf{R_U} \end{gathered} \tag{28}$$

Eq. (28) shows that Eq. (20) is actually just a preconditioned version of Eq. (18), that can be generically written as

$$(\mathbf{M}\mathbf{A_U})(\mathbf{B}d\mathbf{V}) = \mathbf{M}\mathbf{R_U} \tag{29}$$

where $\mathbf{M}$ is the left preconditioner, $\frac{\partial \mathbf{R_V}}{\partial \mathbf{R_U}}$, $\mathbf{B}$ is the right preconditioner, $\frac{\partial \mathbf{U}}{\partial \mathbf{V}}$, and $\mathbf{A_U}$ it the jacobian matrix for the fully coupled system, $\frac{\partial \mathbf{R_U}}{\partial \mathbf{U}}$. This is crucial towards the understanding of the adjoint system of equations, since the transpose operation will reverse the order of operations of these matrix products. Based on Eq. (29), the jacobian for the system based on $\mathbf{R_V}$ and $\mathbf{V}$, denoted as $\mathbf{A_V}$, can be written as

$$\mathbf{A_V} = \mathbf{M}\mathbf{A_U}\mathbf{B} \tag{30}$$

along with its tranpose

$$\mathbf{A_V}^T = (\mathbf{M}\mathbf{A_U}\mathbf{B})^T = \mathbf{B}^T\mathbf{A_U}^T\mathbf{M}^T \tag{31}$$

Thus, in the adjoint $\mathbf{B}$ becomes the left preconditioner, and $\mathbf{M}$ becomes the right preconditioner

$$\begin{gathered} \left(\frac{\partial \mathbf{R_V}}{\partial \mathbf{V}}\right)^T \Lambda_{\mathbf{V}} = -\frac{\partial f}{\partial \mathbf{V}} \\ \left(\frac{\partial \mathbf{U}}{\partial \mathbf{V}}\right)^T \left(\frac{\partial \mathbf{R_U}}{\partial \mathbf{U}}\right)^T \left(\frac{\partial \mathbf{R_V}}{\partial \mathbf{R_U}}\right)^T \Lambda_{\mathbf{V}} = -\left(\frac{\partial \mathbf{U}}{\partial \mathbf{V}}\right)^T \left(\frac{\partial f}{\partial \mathbf{V}}\right) \end{gathered} \tag{32}$$

Based on Eq. (32), it is possible to reuse the exact jacobian of the fully coupled scheme, $\mathbf{A_U}$, instead of computing the exact jacobian of the decoupled system, $\mathbf{A_V}$. This is very attractive, since the implementation of the fully coupled scheme does not need to be changed at the low-level linearizations. Instead, the residual of the adjoint can be formed in the exact same fashion as the fully coupled scheme, and a series of matrix operations can then be performed to transform the equations and dependent variables into those used by the decoupled scheme.

The exact same preconditioners used by the flow solver can be transposed and used to solve the linear system of equations in the adjoint. This is done in two steps and in reverse order of the iterative mechanism used in the flow solver. First, the adjoint costate variables associated with the species mass equations, Λ_{ρ_s}, are solved for

$$\left(\frac{V}{\Delta t}\mathbf{I} + \mathbf{A}_d\right) d\Lambda_{\rho_s} = -\left(\sum_{i=1}^{N_s} \frac{\partial \mathbf{R}'_{\rho_i}}{\partial c_s}\Lambda_{\rho_i} + \frac{\partial \mathbf{R}_\rho}{\partial c_s}\Lambda_\rho + \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial c_s}\Lambda_{\rho\mathbf{u}} + \frac{\partial \mathbf{R}_{\rho E}}{\partial c_s}\Lambda_{\rho E} + \frac{\partial f}{\partial c_s}\right) \tag{33}$$

Followed by the adjoint costate variables associated with the mixture equations, Λ_ρ, $\Lambda_{\rho\mathbf{u}}$, and $\Lambda_{\rho E}$

$$\left(\frac{V}{\Delta t}\mathbf{I} + \mathbf{A}_m\right)\begin{pmatrix} d\Lambda_\rho \\ d\Lambda_{\rho\mathbf{u}} \\ d\Lambda_{\rho E}\end{pmatrix} = -\begin{pmatrix} \sum_{i=1}^{N_s} \frac{\partial \mathbf{R}'_{\rho_i}}{\partial \rho}\Lambda_{\rho_i} + \frac{\partial \mathbf{R}_\rho}{\partial \rho}\Lambda_\rho + \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho}\Lambda_{\rho\mathbf{u}} + \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho}\Lambda_{\rho E} + \frac{\partial f}{\partial \rho} \\ \sum_{i=1}^{N_s} \frac{\partial \mathbf{R}'_{\rho_i}}{\partial \rho\mathbf{u}}\Lambda_{\rho_i} + \frac{\partial \mathbf{R}_\rho}{\partial \rho\mathbf{u}}\Lambda_\rho + \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho\mathbf{u}}\Lambda_{\rho\mathbf{u}} + \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho\mathbf{u}}\Lambda_{\rho E} + \frac{\partial f}{\partial \rho\mathbf{u}} \\ \sum_{i=1}^{N_s} \frac{\partial \mathbf{R}'_{\rho_i}}{\partial \rho E}\Lambda_{\rho_i} + \frac{\partial \mathbf{R}_\rho}{\partial \rho E}\Lambda_\rho + \frac{\partial \mathbf{R}_{\rho\mathbf{u}}}{\partial \rho E}\Lambda_{\rho\mathbf{u}} + \frac{\partial \mathbf{R}_{\rho E}}{\partial \rho E}\Lambda_{\rho E} + \frac{\partial f}{\partial \rho E}\end{pmatrix} \tag{34}$$