Mesh Movement

The volume mesh points are moved by the RBF points which are determined by the surface points. The surface points are parametrized through the design variables. Therefore, the volume mesh points are a function of the design variables.

$$\mathbf{x_{vol}} = \mathbf{x_{vol}}(\mathbf{x_{rbf}}(\mathbf{x_{surf}}(\boldsymbol{\alpha}))) = \mathbf{x_{vol}}(\boldsymbol{\alpha}) \tag{1}$$

The RBF method has the form in Equation 2, which can be written in a system of linear equation. The weights can be solved by using the displacement of the RBF points as shown in Equation 3. The displacements of the volume mesh points are found using weights as shown in Equation 4.

$$f(x) = \sum_{i=1}^{n} w_i \phi(\|x - x_i\|) \tag{2}$$

$$\Delta\mathbf{x_{rbf}} = \mathbf{M}\mathbf{w} \tag{3}$$

$$\Delta\mathbf{x_{rbf}} = \mathbf{A}\mathbf{w} = \mathbf{A}\left[\mathbf{M}\right]^{-1}\Delta\mathbf{x_{rbf}} \tag{4}$$

Since every processor has all the necessary information to move its own volume points, the mesh deformation can be done fully in parallel. Finally, it is possible to define the mesh sensitivities with Equation 5 & 6.

$$\frac{d\mathbf{x_{vol}}}{d\mathbf{x_{rbf}}} = \frac{\Delta\mathbf{x_{vol}}}{\Delta\mathbf{x_{rbf}}} = \mathbf{A}\left[\mathbf{M}\right]^{-1} \tag{5}$$

$$\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} = \frac{d\mathbf{x_{vol}}}{d\mathbf{x_{rbf}}}\frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}}\frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}} = \mathbf{A}\left[\mathbf{M}\right]^{-1}\frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}}\frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}} \tag{6}$$

First-Order Sensitivities

Flow Sensitivities

The cost function L in Equation 7 is a function of the flow state variables $\mathbf{w}$ and the geometry $\mathbf{x_{vol}}$. The state variables are constrained by the steady-state solution of the Navier-Stokes, where the residual is zero as shown in Equation 8.

$$L = L(\mathbf{w}, \mathbf{x_{vol}}) \tag{7}$$

$$\mathbf{R} = \mathbf{R}(\mathbf{w}, \mathbf{x_{vol}}) = \mathbf{0} \tag{8}$$

The gradient of the cost function and the flow residual are defined through the chain rule in Equation 9 & 10.

$$\frac{dL(\mathbf{w}, \mathbf{x_{vol}})}{d\boldsymbol{\alpha}} = \frac{\partial L}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \tag{9}$$

$$\frac{d\mathbf{R}(\mathbf{w},\mathbf{x_{vol}})}{d\boldsymbol{\alpha}} = \frac{\partial \mathbf{R}}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} = \mathbf{0} \tag{10}$$

Direct Differentiation

Equation 10 is used to compute the derivative of the state variables with respect to the design variables $d\mathbf{w}/d\boldsymbol{\alpha}$. The Jacobian of the residual is required and the linear system is solved for N_{des} RHS vectors.

$$\begin{aligned} \frac{\partial \mathbf{R}}{\partial \mathbf{w}} \qquad\quad \frac{d\mathbf{w}}{d\boldsymbol{\alpha}} \qquad\quad &= -\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \qquad \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \\ [N_{cell}\times N_{cell}][N_{cell}\times N_{des}] &= [N_{cell}\times N_{xvol}][N_{xvol}\times N_{des}] \end{aligned} \tag{11}$$

Adjoint Variable

It is possible to augment the gradient of the cost function with an adjoint variable that multiplies the gradient of residual since it is zero. Equation 12 shows the augmented cost function being re-arranged into flow and metric contributions.

$$\begin{aligned} \frac{dL_a(\mathbf{w},\mathbf{x_{vol}})}{d\boldsymbol{\alpha}} &= \frac{dL(\mathbf{w},\mathbf{x_{vol}})}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\frac{d\mathbf{R}(\mathbf{w},\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}) \\ &= \frac{\partial L}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right] \\ &= \underbrace{\left[\frac{\partial L}{\partial \mathbf{w}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}}_{\text{Flow Contributions}} + \underbrace{\left[\frac{\partial L}{\partial \mathbf{x_{vol}}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\right]\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}}_{\text{Metric Contributions}} \end{aligned} \tag{12}$$

The goal of the adjoint variable is to avoid computing the expensive sensitivities by transferring their weights into cheaper sensitivities. In the case of the case above, the mesh sensitivities $d\mathbf{x_{vol}}/d\boldsymbol{\alpha}$ have simple analytical formulas, whereas $d\mathbf{w}/d\boldsymbol{\alpha}$ requires solving Equation 11 Therefore, the adjoint defined such that the flow contribution is zero by solving Equation 13.

$$\begin{aligned} \mathbf{R}^{\psi} &= \frac{\partial L}{\partial \mathbf{w}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{w}} = \mathbf{0} \\ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]^T \qquad \boldsymbol{\psi} \qquad &= \left[\frac{\partial L}{\partial \mathbf{w}}\right]^T \\ [N_{cell}\times N_{cell}][N_{cell}\times 1] &= [N_{cell}\times 1] \end{aligned} \tag{13}$$

Note that solving Equation 13 requires the solution of a linear system with only 1 RHS vector as opposed to N_{des} for the direct differentiation method. After solving for the adjoint, the gradient of the cost function becomes Equation 14.

$$\frac{dL_a}{d\boldsymbol{\alpha}} = \left[\frac{\partial L}{\partial \mathbf{x_{vol}}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\right]\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \tag{14}$$

Mesh Sensitivities

The computation of the mesh sensitivities can be done once before the start of the design cycles since the mesh is always deformed from its initial shape. The matrix $\mathbf{A}$ and $\mathbf{M}$ are constant throughout the design process. However, as shown in Equation 15, the memory required to hold those matrices can be excessive. For this reason, $\mathbf{A}$ is never stored and lazy evaluation is required.

Unfortunately, the factorization of $\mathbf{M}$ is required by every processor. Typical number of RBF points used is in the range of $2,000-10,000$. Note that $12,000$ RBF points will require 1.1 Gb of storage in each processor. Also, at every design cycle, the multiplication of $\mathbf{A}$ has to be done with a matrix with N_{des} columns.

$$\begin{aligned} \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} &= \mathbf{A} \qquad [\mathbf{M}]^{-1} \qquad \frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}} \qquad \frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}} \\ [N_{xvol} N_{des}] &= [N_{xvol} \times N_{rbf}][N_{rbf} \times N_{rbf}][N_{rbf} \times N_{surf}][N_{surf} \times N_{des}] \end{aligned} \tag{15}$$

One way to reduce CPU time of the computation of the gradient is to introduce another adjoint variable. This time, the cost function is augmented in Equation 17 by the mesh deformation residual in 16, which come directly from Equation 15.

$$\mathbf{R^x} = \mathbf{R^x}(\mathbf{x_{vol}}) = \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} - \mathbf{A}\,[\mathbf{M}]^{-1} \frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}} \frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}} = \mathbf{0} \tag{16}$$

$$\begin{aligned} \frac{dL_a(\mathbf{w}, \mathbf{x_{vol}})}{d\boldsymbol{\alpha}} &= \frac{dL(\mathbf{w}, \mathbf{x_{vol}})}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T \frac{d\mathbf{R}(\mathbf{w}, \mathbf{x_{vol}}}{d\boldsymbol{\alpha}}) + \boldsymbol{\lambda}^T \frac{d\mathbf{R^x}(\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}) \\ &= \left[\frac{\partial L}{\partial \mathbf{w}} + \boldsymbol{\psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right] \frac{d\mathbf{w}}{d\boldsymbol{\alpha}} \\ &\quad + \left[\frac{\partial L}{\partial \mathbf{x_{vol}}} + \boldsymbol{\psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} + \boldsymbol{\lambda}^T\right] \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \\ &\quad - \boldsymbol{\lambda}^T \left[\mathbf{A}\,[\mathbf{M}]^{-1} \frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}} \frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}}\right] \end{aligned} \tag{17}$$

First, the flow adjoint is solved as Equation 13. Second, the mesh adjoint can easily be solved in Equation 18 as the sum of two vectors to avoid $d\mathbf{x_{surf}}/d\boldsymbol{\alpha}$.

$$\begin{aligned} \boldsymbol{\lambda}^T &= -(\frac{\partial L}{\partial \mathbf{x_{vol}}} \quad + \boldsymbol{\psi}^T \qquad \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}) \\ [1 \times N_{xvol}] &= \quad [1 \times N_{xvol}] + [1 \times N_{cell}][N_{cell} \times N_{xvol}] \end{aligned} \tag{18}$$

After both adjoint variables are solved, the gradient of the functional can be evaluated as Equation 19. Note that it is possible to take transpose of the gradient in order to solve a smaller system of equation.

$$\frac{dL_a}{d\boldsymbol{\alpha}} = -\boldsymbol{\lambda}^T \mathbf{A}\,[\mathbf{M}]^{-1} \frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}} \frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}} \tag{19}$$

Equation 20 shows that the $\mathbf{A}$ matrix multiplies a vector with 1 column as opposed to N_{des} and the $\mathbf{M}^T$ solves for 1 column instead of N_{des}. Therefore, the calculation of the gradient is now completely independent of the number of design variables.

$$\left[\frac{dL_a}{d\boldsymbol{\alpha}}\right]^T = -\left[\frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}}\right]^T \left[\frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}}\right]^T [\mathbf{M}]^{-T} [\mathbf{A}]^T \boldsymbol{\lambda} = -\left[\frac{d\mathbf{x_{surf}}}{d\boldsymbol{\alpha}}\right]^T \left[\frac{d\mathbf{x_{rbf}}}{d\mathbf{x_{surf}}}\right]^T \mathbf{b} \tag{20}$$

$$\underset{[N_{rbf}\times N_{rbf}]}{[\mathbf{M}]^T}\underset{[N_{rbf}\times 1]}{\mathbf{b}} = \underset{[N_{rbf}\times N_{xvol}]}{[\mathbf{A}]^T}\underset{[N_{xvol}\times 1]}{\boldsymbol{\lambda}} \tag{21}$$

Second-Order Sensitivities

The analytical evaluation of the Hessian has been derived by Papadimitriou and Giannokoglou. The four different ways uses a combination of direct method and adjoint variable for the evaluation of the first and second derivatives.

- Direct-Direct (DD): $N_{des} + N_{des}(N_{des}+1)/2$
- Adjoint-Direct (AD): $2N_{des} + 1$
- Adjoint-Adjoint (AA):$2N_{des} + 1$
- Direct-Adjoint (DA):N_{des}

Direct-Direct

The direct-direct method uses the direct differentiation method for the first derivative as shown in Equation 22 & 23.

$$\frac{dL(\mathbf{w},\mathbf{x_{vol}})}{d\boldsymbol{\alpha}} = \frac{\partial L}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \tag{22}$$

$$\frac{d\mathbf{R}(\mathbf{w},\mathbf{x_{vol}})}{d\boldsymbol{\alpha}} = \frac{\partial \mathbf{R}}{\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} = \mathbf{0} \tag{23}$$

The full formulation of the Hessian of the cost function is shown in Equation 24 with its matrix sizes shown in Equation 25. The term $d\mathbf{w}/d\boldsymbol{\alpha}$ requires the solution of Equation 11, which requires N_{des} system evaluations.

$$\begin{aligned}\frac{d^2L}{d\boldsymbol{\alpha}^2} = &\left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{w}^2}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{w}}\frac{d^2\mathbf{w}}{d\boldsymbol{\alpha}^2} \\ &+ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}}\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}}^2}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d^2\mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2}\end{aligned} \tag{24}$$

$$\begin{aligned}[N_{des}\times N_{des}] =&[N_{des}\times N_{cell}][N_{cell}\times N_{xvol}][N_{xvol}\times N_{des}] \\ &+ [N_{des}\times N_{cell}][N_{cell}\times N_{cell}][N_{cell}\times N_{des}] \\ &+ [1\times N_{cell}][N_{cell}\times N_{des}\times N_{des}] \\ &+ [N_{des}\times N_{xvol}][N_{xvol}\times N_{cell}][N_{cell}\times N_{des}] \\ &+ [N_{des}\times N_{xvol}][N_{xvol}\times N_{xvol}][N_{xvol}\times N_{des}] \\ &+ [1\times N_{xvol}][N_{xvol}\times N_{des}\times N_{des}]\end{aligned} \tag{25}$$

The term $d^2\mathbf{w}/d\boldsymbol{\alpha}^2$ can be found in the second-order direct-differentiation of the flow residual. The term requires the solution of Equation 27, which requires $N_{des}(N_{des}+1)/2$ system evaluations.

$$\begin{aligned}\frac{d^2\mathbf{R}}{d\boldsymbol{\alpha}^2} = &\left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{w}}\frac{d^2\mathbf{w}}{d\boldsymbol{\alpha}^2} \\ &+ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}^2}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d^2\mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} = \mathbf{0}\end{aligned} \tag{26}$$

$$\begin{aligned}\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\frac{d^2\mathbf{w}}{d\boldsymbol{\alpha}^2} = -\Bigg(&\left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} \\ &+ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}^2}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d^2\mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2}\Bigg)\end{aligned} \tag{27}$$

$$[N_{cell}\times N_{cell}][N_{cell}\times N_{des}\times N_{des}] = [N_{cell}\times N_{des}\times N_{des}] \tag{28}$$

A total of $N_{des} + N_{des}(N_{des}+1)/2$ system evaluations are required.

Adjoint-Direct

The adjoint-direct method starts with the gradient of the augmented cost function derived from the adjoint in Equation 29. It is then differentiated directly to give Equation 30.

$$\frac{dL_a}{d\boldsymbol{\alpha}} = \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \tag{29}$$

$$\begin{aligned}\frac{d^2L_a}{d\boldsymbol{\alpha}^2} = & \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}}^2}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}}\partial \mathbf{w}}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \frac{\partial L}{\partial \mathbf{x_{vol}}}\frac{d^2\mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} \\ & + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{d\boldsymbol{\psi}^T}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \left(\boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}^2}\right)\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \\ & + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \left(\boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}\partial \mathbf{w}}\right)\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}}\frac{d^2\mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2}\end{aligned} \tag{30}$$

The first order flow sensitivities $d\mathbf{w}/d\boldsymbol{\alpha}$ are evaluated from Equation 11 and require N_{des} system evaluations. The adjoint variable is evaluated in Equation 13 at the cost of 1 system evaluation and is the reason Equation 29 holds true.

That leaves $d\boldsymbol{\psi}^T/d\boldsymbol{\alpha}$ to be evaluated. The term can be found in the direct differentiation of the adjoint residual giving Equation 31. Solving Equation 32 costs N_{des} system evaluations.

$$\begin{aligned}\frac{d\mathbf{R}^{\psi}}{d\boldsymbol{\alpha}} = & \frac{\partial^2 L}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \frac{\partial^2 L}{\partial \mathbf{w}^2}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]^T \frac{d\boldsymbol{\psi}^T}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} \\ = & \left[\frac{\partial^2 L}{\partial \mathbf{w}\partial \mathbf{x_{vol}}} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\right]\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{\partial^2 L}{\partial \mathbf{w}^2} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\right]\frac{d\mathbf{w}}{d\boldsymbol{\alpha}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]^T \frac{d\boldsymbol{\psi}^T}{d\boldsymbol{\alpha}} = \mathbf{0}\end{aligned} \tag{31}$$

$$\underbrace{\left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]^T \frac{d\boldsymbol{\psi}^T}{d\boldsymbol{\alpha}}}_{[N_{cell}\times N_{cell}][N_{cell}\times N_{des}]} \; = \; - \underbrace{\left(\left[\frac{\partial^2 L}{\partial \mathbf{w}\partial \mathbf{x_{vol}}} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}\partial \mathbf{x_{vol}}}\right]\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{\partial^2 L}{\partial \mathbf{w}^2} + \boldsymbol{\psi}^T\frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\right]\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right)}_{[N_{cell}\times N_{des}]} \tag{32}$$

A total of $2N_{des}+1$ system evaluations are required to compute the Hessian using the adjoint-direct approach.

Adjoint-Adjoint

Looking at the previous method, it is possible to add adjoint variables to eliminate some expensive terms by augmenting derivative of the augmented cost function like in Equation 30.

$$\frac{d^2 L_a^*}{d\boldsymbol{\alpha}^2} = \frac{d^2 L_a}{d\boldsymbol{\alpha}^2} + \boldsymbol{\beta}^T \frac{d\mathbf{R}}{d\boldsymbol{\alpha}} + \boldsymbol{\gamma}^T \frac{d\mathbf{R}^{\psi}}{d\boldsymbol{\alpha}} \tag{33}$$

The expression can be fully expanded by inserting Equation 30, 10 and 31 into Equation 33. The terms are then factored and gives Equation 34

$$\begin{aligned}
\frac{d^2 L_a^*}{d\boldsymbol{\alpha}^2} =& \frac{\partial L}{\partial \mathbf{x_{vol}}} \frac{d^2 \mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} + \boldsymbol{\psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \frac{d^2 \mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} \\
&+ \left\{ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial {\mathbf{x_{vol}}}^2} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \left(\boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial {\mathbf{x_{vol}}}^2}\right) + \boldsymbol{\beta}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \right. \\
&\quad \left. + \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \boldsymbol{\gamma}^T \frac{\partial^2 L}{\partial \mathbf{w} \partial \mathbf{x_{vol}}} + \boldsymbol{\gamma}^T \boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w} \partial \mathbf{x_{vol}}} \right\} \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \\
&+ \left\{ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}} \partial \mathbf{w}} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \left(\boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}} \partial \mathbf{w}}\right) \right. \\
&\quad \left. + \boldsymbol{\beta}^T \frac{\partial \mathbf{R}}{\partial \mathbf{w}} + \boldsymbol{\gamma}^T \frac{\partial^2 L}{\partial \mathbf{w}^2} + \boldsymbol{\gamma}^T \left(\boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w}^2}\right) \right\} \frac{d\mathbf{w}}{d\boldsymbol{\alpha}} \\
&+ \left\{ \left[\frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T + \boldsymbol{\gamma}^T \left[\frac{\partial \mathbf{R}}{\partial \mathbf{w}}\right]^T \right\} \frac{d\boldsymbol{\psi}^T}{d\boldsymbol{\alpha}}
\end{aligned} \tag{34}$$

The derivative of the flow adjoint can be eliminated by defining $\boldsymbol{\gamma}$ to make the last term zero. Unfortunately, as seen in Equation 35, the cost of eliminating $d\boldsymbol{\psi}^T/d\boldsymbol{\alpha}$ is the same as solving for it. Evaluating $\boldsymbol{\gamma}$ costs N_{des} system evaluations.

$$\begin{aligned}
\frac{\partial \mathbf{R}}{\partial \mathbf{w}} \qquad\qquad \boldsymbol{\gamma} \qquad\qquad &= \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \qquad\qquad \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \\
[N_{cell} \times N_{cell}][N_{cell} \times N_{des}] &= [N_{cell} \times N_{xvol}][N_{xvol} \times N_{des}]
\end{aligned} \tag{35}$$

The same unfortunate scenario happens for $d\mathbf{w}/d\boldsymbol{\alpha}$ where eliminating it costs N_{des} flow evaluations as seen in Equation 36

$$\begin{aligned}
\frac{\partial \mathbf{R}}{\partial \mathbf{w}}^T \qquad\qquad \boldsymbol{\beta} \qquad\qquad &= -\left\{ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}\right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}} \partial \mathbf{w}} + \ldots \right\}^T \\
[N_{cell} \times N_{cell}][N_{cell} \times N_{des}] &= \qquad\qquad [N_{cell} \times N_{des}]
\end{aligned} \tag{36}$$

Finally, the adjoint-adjoint Hessian after solving for all the adjoint variables reduces to Equation 37.

$$
\begin{aligned}
\frac{d^2 L_a^*}{d\boldsymbol{\alpha}^2} =& \frac{\partial L}{\partial \mathbf{x_{vol}}} \frac{d^2 \mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} + \boldsymbol{\psi}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \frac{d^2 \mathbf{x_{vol}}}{d\boldsymbol{\alpha}^2} \\
&+ \Bigg\{ \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \right]^T \frac{\partial^2 L}{\partial \mathbf{x_{vol}}^2} + \left[\frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \right]^T \left(\boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{x_{vol}}^2} \right) + \boldsymbol{\beta}^T \frac{\partial \mathbf{R}}{\partial \mathbf{x_{vol}}} \\
&\qquad + \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}} \boldsymbol{\gamma}^T \frac{\partial^2 L}{\partial \mathbf{w} \partial \mathbf{x_{vol}}} + \boldsymbol{\gamma}^T \boldsymbol{\psi}^T \frac{\partial^2 \mathbf{R}}{\partial \mathbf{w} \partial \mathbf{x_{vol}}} \Bigg\} \frac{d\mathbf{x_{vol}}}{d\boldsymbol{\alpha}}
\end{aligned} \tag{37}
$$

A total of $2N_{des} + 1$ system evaluations are required to solve every adjoint.

Direct-Adjoint

The direct-adjoint method is directly linked to the direct-direct approach. The Hessian of the cost function expression is augmented with the Hessian of the flow residual as seen in Equation 38. Equation 24 & 26.

$$\frac{d^2L^{**}}{d\boldsymbol{\alpha}^2} = \frac{d^2L}{d\boldsymbol{\alpha}^2} + \boldsymbol{\psi}^T\frac{d^2\mathbf{R}}{d\boldsymbol{\alpha}^2} \tag{38}$$

$$\begin{aligned}\frac{d^2L**}{d\boldsymbol{\alpha}^2} = & \left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T\left\{\frac{\partial^2L}{\partial\mathbf{w}\partial\mathbf{x}_{\mathbf{vol}}} + \boldsymbol{\psi}^T\frac{\partial^2\mathbf{R}}{\partial\mathbf{w}\partial\mathbf{x}_{\mathbf{vol}}}\right\}\frac{d\mathbf{x}_{\mathbf{vol}}}{d\boldsymbol{\alpha}} + \left[\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\right]^T\left\{\frac{\partial^2L}{\partial\mathbf{w}^2} + \boldsymbol{\psi}^T\frac{\partial^2\mathbf{R}}{\partial\mathbf{w}^2}\right\}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\\ & + \left\{\frac{\partial L}{\partial\mathbf{w}} + \boldsymbol{\psi}^T\frac{\partial\mathbf{R}}{\partial\mathbf{w}}\right\}\frac{d^2\mathbf{w}}{d\boldsymbol{\alpha}^2} + \left[\frac{d\mathbf{x}_{\mathbf{vol}}}{d\boldsymbol{\alpha}}\right]^T\left\{\frac{\partial^2L}{\partial\mathbf{x}_{\mathbf{vol}}\partial\mathbf{w}} + \boldsymbol{\psi}^T\frac{\partial^2\mathbf{R}}{\partial\mathbf{x}_{\mathbf{vol}}\partial\mathbf{w}}\right\}\frac{d\mathbf{w}}{d\boldsymbol{\alpha}}\\ & + \left[\frac{d\mathbf{x}_{\mathbf{vol}}}{d\boldsymbol{\alpha}}\right]^T\left\{\frac{\partial^2L}{\partial{\mathbf{x}_{\mathbf{vol}}}^2} + \boldsymbol{\psi}^T\frac{\partial^2\mathbf{R}}{\partial{\mathbf{x}_{\mathbf{vol}}}^2}\right\}\frac{d\mathbf{x}_{\mathbf{vol}}}{d\boldsymbol{\alpha}} + \left\{\frac{\partial L}{\partial\mathbf{x}_{\mathbf{vol}}} + \boldsymbol{\psi}^T\frac{\partial\mathbf{R}}{\partial\mathbf{x}_{\mathbf{vol}}}\right\}\frac{d^2\mathbf{x}_{\mathbf{vol}}}{d\boldsymbol{\alpha}^2}\end{aligned} \tag{39}$$

Looking at Equation 39, the expensive $d^2\mathbf{w}/d\boldsymbol{\alpha}^2$ term can now be ignored by solving the adjoint. Furthermore, it only requires 1 system evaluation as seen in Equation 13. The first-order flow sensitivities still have to be solved at the cost of N_{des} from Equation 11. Therefore, the total cost of $N_{des}+1$ system evaluations are required, making it the cheapest of the four methods.