Time Dependent Adjoint Sensitivities for Second-Order Systems

Komahan Boopathy *and* **Graeme J. Kennedy**

June 20, 2018

Part I

Adjoint Sensitivities

Chapter 1

Discrete Adjoint Formulations

1.1 Backwards Difference Formulae

1.2 Newmark–Beta–Gamma Method

The second–order governing differential equations are posed in the following descriptor form at the kth time step:

$$R_k(\ddot{q}_k, \dot{q}_k, q_k, t_k, x) = 0.$$

We use Newmark–Beta–Gamma (NBG) method to approximate the states:

$$S_k = \dot{q}_{k-1} + (1-\gamma)h\ddot{q}_{k-1} + \gamma h\ddot{q}_k - \dot{q}_k$$

$$T_k = q_{k-1} + h\dot{q}_{k-1} + \frac{1-2\beta}{2}h^2\ddot{q}_{k-1} + \beta h^2\ddot{q}_k - q_k.$$

The acceleration states $\ddot{q}_k$ are the primary unknown at each time step. We introduce λ_k, ψ_k and ϕ_k as adjoint variables associated with each of these equations. The Lagrangian function is written as:

$$\mathcal{L} = \sum_{k=0}^{N} hf_k(\underline{\ddot{q}_k}, \dot{q}_k, q_k, x) + \sum_{k=0}^{N} h\lambda_k^T R_k(\underline{\ddot{q}_k}, \dot{q}_k, q_k, x) + \sum_{k=0}^{N} \psi_k^T S_k(\underline{\dot{q}_k}, \dot{q}_{k-1}, \ddot{q}_{k-1}, \ddot{q}_k) + \sum_{k=0}^{N} \phi_k^T T_k(\underline{q_k}, q_{k-1}, \ddot{q}_{k-1}, \ddot{q}_k).$$

The underlined variables denote the primary unknown in each equation. The stationary points of the Lagrangian function with respect to the state variables can be used to determine the adjoint variables.

Solving for ϕ: Setting $\dfrac{\partial \mathcal{L}}{\partial q_k} = 0$ yields,

$$\phi_k = \phi_{k+1} + h\left\{\frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T + h\left[\frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1}. \tag{1.1}$$

Solving for ψ: Setting $\dfrac{\partial \mathcal{L}}{\partial \dot{q}_k} = 0$ yields,

$$\psi_k = \psi_{k+1} + h\phi_{k+1} + h\left\{\frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + h\frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T + h\left[\frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + h\frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1}. \tag{1.2}$$

Solving for λ: Setting $\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_k} = 0$ yields,

$$
\begin{aligned}
\left[\frac{\partial R_k}{\partial \ddot{q}_k} + \gamma h \frac{\partial R_k}{\partial \dot{q}_k} + \beta h^2 \frac{\partial R_k}{\partial q_k}\right]^T \lambda_k = &- \left\{\frac{\partial f_k}{\partial \ddot{q}_k} + \gamma h \frac{\partial f_k}{\partial \dot{q}_k} + \beta h^2 \frac{\partial f_k}{\partial q_k}\right\}^T \\
&- \frac{1}{h}\left\{\gamma h \psi_k + \beta h^2 \phi_k\right\}^T \\
&- \left\{(1-\gamma) h \frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T \\
&- \left[(1-\gamma) h \frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + \frac{1-2\beta}{2} h^2 \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \\
&- \frac{1}{h}\left\{(1-\gamma) h \psi_{k+1} + \frac{1-2\beta}{2} h^2 \phi_{k+1}\right\}^T .
\end{aligned}
\tag{1.3}
$$

We can equivalently scale the equation with $1/h^2$ and represent as follows,

$$
\begin{aligned}
\left[\frac{1}{h^2}\frac{\partial R_k}{\partial \ddot{q}_k} + \gamma \frac{1}{h} \frac{\partial R_k}{\partial \dot{q}_k} + \beta \frac{\partial R_k}{\partial q_k}\right]^T \lambda_k = &- \left\{\frac{1}{h^2}\frac{\partial f_k}{\partial \ddot{q}_k} + \gamma \frac{1}{h} \frac{\partial f_k}{\partial \dot{q}_k} + \beta \frac{\partial f_k}{\partial q_k}\right\}^T \\
&- \frac{1}{h}\left\{\gamma \frac{1}{h} \psi_k + \beta \phi_k\right\}^T \\
&- \left\{(1-\gamma) \frac{1}{h} \frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + \frac{1-2\beta}{2} \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T \\
&- \left[(1-\gamma) \frac{1}{h} \frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + \frac{1-2\beta}{2} \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \\
&- \frac{1}{h}\left\{(1-\gamma) \frac{1}{h} \psi_{k+1} + \frac{1-2\beta}{2} \phi_{k+1}\right\}^T .
\end{aligned}
\tag{1.4}
$$

Grouping the terms together we get,

$$
\begin{aligned}
\left[\frac{1}{h^2}\frac{\partial R_k}{\partial \ddot{q}_k} + \gamma \frac{1}{h} \frac{\partial R_k}{\partial \dot{q}_k} + \beta \frac{\partial R_k}{\partial q_k}\right]^T \lambda_k = &- \left\{\frac{1}{h^2}\frac{\partial f_k}{\partial \ddot{q}_k} + \gamma \frac{1}{h} \frac{\partial f_k}{\partial \dot{q}_k} + \beta \frac{\partial f_k}{\partial q_k}\right\}^T \\
&- \left\{\gamma \frac{1}{h} \frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + \gamma \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T \\
&- \left[\gamma \frac{1}{h} \frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + \gamma \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \\
&- \left\{\beta \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T \\
&- \left[\beta \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \\
&- \left\{(1-\gamma) \frac{1}{h} \frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + (\frac{1}{2} - \beta) \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T \\
&- \left[(1-\gamma) \frac{1}{h} \frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + (\frac{1}{2} - \beta) \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \\
&- \frac{1}{h}\left\{\frac{1}{h} \psi_{k+1} + (\frac{1}{2} + \gamma) \phi_{k+1}\right\}^T .
\end{aligned}
\tag{1.5}
$$

$$\left[\frac{1}{h^2}\frac{\partial R_k}{\partial \ddot{q}_k} + \gamma\frac{1}{h}\frac{\partial R_k}{\partial \dot{q}_k} + \beta\frac{\partial R_k}{\partial q_k}\right]^T \lambda_k = - \left\{\frac{1}{h^2}\frac{\partial f_k}{\partial \ddot{q}_k} + \gamma\frac{1}{h}\frac{\partial f_k}{\partial \dot{q}_k} + \beta\frac{\partial f_k}{\partial q_k}\right\}^T$$
$$- \left\{\frac{1}{h}\frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + (\frac{1}{2}+\gamma)\frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T$$
$$- \left[\frac{1}{h}\frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + (\frac{1}{2}+\gamma)\frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} \tag{1.6}$$
$$- \frac{1}{h}\left\{\frac{1}{h}\psi_{k+1} + (\frac{1}{2}+\gamma)\phi_{k+1}\right\}^T$$

The total derivative can be computed as follows:

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial F}{\partial x} = \sum_{k=0}^{N} h\frac{\partial f_k}{\partial x}^T + \sum_{k=0}^{N} h\frac{\partial R_k}{\partial x}^T \lambda_k.$$

1.3 Adams–Bashforth–Moulton

The second–order governing differential equations are posed in the following descriptor form at the k-th time step:

$$R_k(\underline{\ddot{q}_k}, \dot{q}_k, q_k, t_k, x) = 0.$$

We use an mth order Adams–Bashforth–Moulton (ABM) method to approximate the states:

$$S_k = \dot{q}_{k-1} + h\sum_{i=0}^{m-1} a_i \ddot{q}_{k-i} - \underline{\dot{q}_k}$$

$$T_k = q_{k-1} + h\sum_{i=0}^{m-1} a_i \dot{q}_{k-i} - \underline{q_k}.$$

The acceleration states $\ddot{q}_k$ are the primary unknown at each time step. We introduce λ_k, ψ_k and ϕ_k as adjoint variables associated with respective equations. The Lagrangian function is written as:

$$\mathcal{L} = \sum_{k=0}^{N} hf_k + \sum_{k=0}^{N} h\lambda_k^T R_k + \sum_{k=0}^{N} \psi_k^T S_k + \sum_{k=0}^{N} \phi_k^T T_k.$$

The stationary point of the Lagrangian yields the set of linear equations for the adjoint system.

1.3.1 First Order ABM

Forward Mode

Step $k = 1$: The initial conditions are q_1, $\dot{q}_1$.

Step $k = 2$: The state variables are determined at this step using the following relations.

$$\dot{q}_2 = \dot{q}_1 + ha_{11}\ddot{q}_2$$
$$q_2 = q_1 + ha_{11}\dot{q}_2$$

$$\begin{array}{c|c|l}
\lambda_2^T & h & R_2(\ddot{q}_2, \dot{q}_1 + ha_{11}\ddot{q}_2, q_1 + ha_{11}\dot{q}_2) \\
 & h & f_2(\ddot{q}_2, \dot{q}_1 + ha_{11}\ddot{q}_2, q_1 + ha_{11}\dot{q}_2) \\
\psi_2^T & & \mathbf{S_2}\,(\dot{q}_1 + ha_{11}\ddot{q}_2 - \dot{q}_2) \\
\phi_2^T & & \mathbf{T_2}\,(q_1 + ha_{11}\dot{q}_2 - q_2)
\end{array}$$

Step $k = 3$**:** The state variables are determined at this step using the following relations.

$$\dot{q}_3 = \dot{q}_2 + ha_{11}\ddot{q}_3$$
$$q_3 = q_2 + ha_{11}\dot{q}_3$$

$$\begin{array}{c|c|l} \lambda_3^T & h & R_3(\ddot{q}_3, \dot{q}_2 + ha_{11}\ddot{q}_3, q_2 + ha_{11}\dot{q}_3) \\ & h & f_3(\ddot{q}_3, \dot{q}_2 + ha_{11}\ddot{q}_3, q_2 + ha_{11}\dot{q}_3) \\ \psi_3^T & & \mathbf{S_3}\,(\dot{q}_2 + ha_{11}\ddot{q}_3 - \dot{q}_3) \\ \phi_3^T & & \mathbf{T_3}\,(q_2 + ha_{11}\dot{q}_3 - q_3) \end{array}$$

Step $k = 4$**:** The state variables are determined at this step using the following relations.

$$\dot{q}_4 = \dot{q}_3 + ha_{11}\ddot{q}_4$$
$$q_4 = q_3 + ha_{11}\dot{q}_4$$

$$\begin{array}{c|c|l} \lambda_4^T & h & R_4(\ddot{q}_4, \dot{q}_3 + ha_{11}\ddot{q}_4, q_3 + ha_{11}\dot{q}_4) \\ & h & f_4(\ddot{q}_4, \dot{q}_3 + ha_{11}\ddot{q}_4, q_3 + ha_{11}\dot{q}_4) \\ \psi_4^T & & \mathbf{S_4}\,(\dot{q}_3 + ha_{11}\ddot{q}_4 - \dot{q}_4) \\ \phi_4^T & & \mathbf{T_4}\,(q_3 + ha_{11}\dot{q}_4 - q_4) \end{array}$$

Reverse Mode

We solve for the adjoint variables starting from the last time step.

Step $k = 4$**:**

- Setting $\dfrac{\partial L}{\partial q_4} = 0$, we get:

$$\frac{\partial T_4}{\partial q_4}^T \phi_4 = 0$$

$$\boxed{\phi_4 = 0}$$

- Setting $\dfrac{\partial L}{\partial \dot{q}_4} = 0$, we get:

$$\frac{\partial S_4}{\partial \dot{q}_4}^T \psi_4 + \frac{\partial T_4}{\partial \dot{q}_4}^T \phi_4 = 0$$

$$\boxed{\psi_4 = 0}$$

- Setting $\dfrac{\partial L}{\partial \ddot{q}_4} = 0$, we get:

$$h\frac{\partial R_4}{\partial \ddot{q}_4}^T \lambda_4 + h\frac{\partial f_4}{\partial \ddot{q}_4}^T + \frac{\partial S_4}{\partial \ddot{q}_4}^T \psi_4 = 0$$

$$\boxed{h\left[\frac{\partial R_4}{\partial \ddot{q}_4} + ha_{11}\frac{\partial R_4}{\partial \dot{q}_4} + h^2a_{11}^2\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial \ddot{q}_4} + ha_{11}\frac{\partial f_4}{\partial \dot{q}_4} + h^2a_{11}^2\frac{\partial f_4}{\partial q_4}\right\}^T + ha_{11}\psi_4 = 0}$$

Step $k = 3$**:**

- Setting $\dfrac{\partial L}{\partial q_3} = 0$, we get:

$$\frac{\partial T_3}{\partial q_3}^T \phi_3 + \frac{\partial T_4}{\partial q_3}^T \phi_4 + h \left[\frac{\partial R_4}{\partial q_3}\right]^T \lambda_4 + h \left\{\frac{\partial f_4}{\partial q_3}\right\}^T = 0$$

$$\boxed{\phi_3 = \phi_4 + h \left[\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h \left\{\frac{\partial f_4}{\partial q_4}\right\}^T}$$

- Setting $\dfrac{\partial L}{\partial \dot{q}_3} = 0$, we get:

$$\frac{\partial S_3}{\partial \dot{q}_3}^T \psi_3 + \frac{\partial T_3}{\partial \dot{q}_3}^T \phi_3 + \frac{\partial S_4}{\partial \dot{q}_3}^T \psi_4 + \frac{\partial T_4}{\partial \dot{q}_3}^T \phi_4 + h \left[\frac{\partial R_4}{\partial \dot{q}_3}\right]^T \lambda_4 + h \left\{\frac{\partial f_4}{\partial \dot{q}_3}\right\}^T = 0$$

$$\boxed{\psi_3 = h a_{11} \phi_3 + \psi_4 + h \left[\frac{\partial R_4}{\partial \dot{q}_4} + h a_{11} \frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h \left\{\frac{\partial f_4}{\partial \dot{q}_4} + h a_{11} \frac{\partial f_4}{\partial q_4}\right\}^T}$$

- Setting $\dfrac{\partial L}{\partial \ddot{q}_3} = 0$, we get:

$$h \frac{\partial R_3}{\partial \ddot{q}_3}^T \lambda_3 + h \frac{\partial f_3}{\partial \ddot{q}_3}^T + \frac{\partial S_3}{\partial \ddot{q}_3}^T \psi_3 = 0$$

$$\boxed{h \left[\frac{\partial R_3}{\partial \ddot{q}_3} + h a_{11} \frac{\partial R_3}{\partial \dot{q}_3} + h^2 a_{11}^2 \frac{\partial R_3}{\partial q_3}\right]^T \lambda_3 + h \left\{\frac{\partial f_3}{\partial \ddot{q}_3} + h a_{11} \frac{\partial f_3}{\partial \dot{q}_3} + h^2 a_{11}^2 \frac{\partial f_3}{\partial q_3}\right\}^T + h a_{11} \psi_3 = 0}$$

General Relations: We can identify the recursive relations based on the above equations.

$$\boxed{\phi_k = \phi_{k+1} + h \left[\frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} + h \left\{\frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T}$$

$$\boxed{\psi_k = h a_{11} \phi_k + \psi_{k+1} + + h \left[\frac{\partial R_{k+1}}{\partial \dot{q}_{k+1}} + h a_{11} \frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} + h \left\{\frac{\partial f_{k+1}}{\partial \dot{q}_{k+1}} + h a_{11} \frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T}$$

$$\boxed{h \left[\frac{\partial R_k}{\partial \ddot{q}_k} + h a_{11} \frac{\partial R_k}{\partial \dot{q}_k} + h^2 a_{11}^2 \frac{\partial R_k}{\partial q_k}\right]^T \lambda_k + h \left\{\frac{\partial f_k}{\partial \ddot{q}_k} + h a_{11} \frac{\partial f_k}{\partial \dot{q}_k} + h^2 a_{11}^2 \frac{\partial f_k}{\partial q_k}\right\}^T + h a_{11} \psi_k = 0}$$

Solve for ϕ: Setting $\dfrac{\partial \mathcal{L}}{\partial q_k} = 0$ yields:

$$\phi_k^T \frac{\partial T_k}{\partial q_k} + \phi_{k+1}^T \frac{\partial T_{k+1}}{\partial q_k} + h\lambda_{k+1}^T \frac{\partial R_{k+1}}{\partial q_k} + h\frac{\partial f_{k+1}}{\partial q_k} = 0$$

which simplifies to

$$\boxed{\phi_k = \phi_{k+1} + h\left[\frac{\partial R_{k+1}}{\partial q_{k+1}}\right]^T \lambda_{k+1} + h\left\{\frac{\partial f_{k+1}}{\partial q_{k+1}}\right\}^T}$$

Solve for ψ: Setting $\dfrac{\partial \mathcal{L}}{\partial \dot{q}_k} = 0$ yields:

$$\psi_k^T \frac{\partial S_k}{\partial \dot{q}_k} + \psi_{k+1}^T \frac{\partial S_{k+1}}{\partial \dot{q}_k} + \sum_{i=0}^{m-1} \phi_{k+i}^T \frac{\partial T_{k+i}}{\partial \dot{q}_k} + h\sum_{i=1}^{m-1} \lambda_{k+i}^T \frac{\partial R_{k+i}}{\partial \dot{q}_k} + h\sum_{i=1}^{m-1} \frac{\partial f_{k+i}}{\partial \dot{q}_k} = 0$$

which simplifies to

$$\psi_k = \psi_{k+1} + h\sum_{i=0}^{m-1} a_i \phi_{k+i} + h\sum_{i=1}^{m-1}\left[\frac{\partial R_{k+i}}{\partial \dot{q}_{k+i}} + \sum_{j=0}^{i} ha_j \frac{\partial R_{k+i}}{\partial q_{k+i}}\right]^T \lambda_{k+1} + h\sum_{i=1}^{m-1}\left\{\frac{\partial f_{k+i}}{\partial \dot{q}_{k+i}} + \sum_{j=0}^{i} ha_j \frac{\partial f_{k+i}}{\partial q_{k+i}}\right\}^T \tag{1.7}$$

Solve for λ: Setting $\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_k} = 0$ yields:

$$h\lambda_k^T \frac{\partial R_k}{\partial \ddot{q}_k} + h\frac{\partial f_k}{\partial \ddot{q}_k} + \sum_{i=1}^{m-1} h\lambda_{k+i}^T \frac{\partial R_{k+i}}{\partial \ddot{q}_k} + \sum_{i=1}^{m-1} h\frac{\partial f_{k+1}}{\partial \ddot{q}_k} + \sum_{i=0}^{m-1} \psi_{k+i}^T \frac{\partial S_{k+i}}{\partial \ddot{q}_k} + \frac{\partial T_{k+i}}{\partial \ddot{q}_k} = 0$$

which simplifies to

$$\begin{aligned}
h\left[\frac{\partial R_k}{\partial \ddot{q}_k} + ha_0\frac{\partial R_k}{\partial \dot{q}_k} + h^2a_0^2\frac{\partial R_k}{\partial q_k}\right]^T \lambda_k = & - h\left\{\frac{\partial R_k}{\partial \ddot{q}_k} + ha_0\frac{\partial R_k}{\partial \dot{q}_k} + h^2a_0^2\frac{\partial R_k}{\partial q_k}\right\}^T \\
& - h\sum_{i=1}^{m-1} h\left[\frac{\partial R_{k+i}}{\partial \dot{q}_{k+i}}\frac{\partial \dot{q}_{k+i}}{\partial \ddot{q}_k} + \frac{\partial R_{k+i}}{\partial q_{k+i}}\frac{\partial q_{k+i}}{\partial \ddot{q}_k}\right]^T \lambda_{k+i} \\
& - h\sum_{i=1}^{m-1} h\left\{\frac{\partial f_{k+i}}{\partial \dot{q}_{k+i}}\frac{\partial \dot{q}_{k+i}}{\partial \ddot{q}_k} + \frac{\partial f_{k+i}}{\partial q_{k+i}}\frac{\partial q_{k+i}}{\partial \ddot{q}_k}\right\}^T \\
& - h\sum_{i=0}^{m-1} ha_i\psi_{k+i} \\
& - h\sum_{i=0}^{m-1} ha_iha_i\psi_{k+i}
\end{aligned} \tag{1.8}$$

1.3.2 Second Order ABM

Forward Mode

Step $k = 1$: The initial conditions are q_1, $\dot{q}_1$.

Step $k = 2$**:** The state variables are determined at this step using the following relations.

$$\dot{q}_2 = \dot{q}_1 + ha_{11}\ddot{q}_2$$
$$q_2 = q_1 + ha_{21}\dot{q}_2 + ha_{22}\dot{q}_1$$

$$\begin{array}{c|c|l} \lambda_2^T & h & R_2(\ddot{q}_2, \dot{q}_1 + ha_{11}\ddot{q}_2, q_1 + ha_{21}\dot{q}_2 + ha_{22}\dot{q}_1) \\ & h & f_2(\ddot{q}_2, \dot{q}_1 + ha_{11}\ddot{q}_2, q_1 + ha_{21}\dot{q}_2 + ha_{22}\dot{q}_1) \\ \psi_2^T & & S_2\left(\dot{q}_1 + ha_{11}\ddot{q}_2 - \dot{q}_2\right) \\ \phi_2^T & & T_2\left(q_1 + ha_{21}\dot{q}_2 + ha_{22}\dot{q}_1 - q_2\right) \end{array}$$

Step $k = 3$**:** The state variables are determined at this step using the following relations.

$$\dot{q}_3 = \dot{q}_2 + ha_{21}\ddot{q}_3 + ha_{22}\ddot{q}_2$$
$$q_3 = q_2 + ha_{21}\dot{q}_3 + ha_{22}\dot{q}_2$$

$$\begin{array}{c|c|l} \lambda_3^T & h & R_3(\ddot{q}_3, \dot{q}_2 + ha_{21}\ddot{q}_3 + ha_{22}\ddot{q}_2, q_2 + ha_{21}\dot{q}_3 + ha_{22}\dot{q}_2) \\ & h & f_3(\ddot{q}_3, \dot{q}_2 + ha_{21}\ddot{q}_3 + ha_{22}\ddot{q}_2, q_2 + ha_{21}\dot{q}_3 + ha_{22}\dot{q}_2) \\ \psi_3^T & & S_3\left(\dot{q}_2 + ha_{21}\ddot{q}_3 + ha_{22}\ddot{q}_2 - \dot{q}_3\right) \\ \phi_3^T & & T_3\left(q_2 + ha_{21}\dot{q}_3 + ha_{22}\dot{q}_2 - q_3\right) \end{array}$$

Step $k = 4$**:** The state variables are determined at this step using the following relations.

$$\dot{q}_4 = \dot{q}_3 + ha_{21}\ddot{q}_4 + ha_{22}\ddot{q}_3$$
$$q_4 = q_3 + ha_{21}\dot{q}_4 + ha_{22}\dot{q}_3$$

$$\begin{array}{c|c|l} \lambda_4^T & h & R_4(\ddot{q}_4, \dot{q}_3 + ha_{21}\ddot{q}_4 + ha_{22}\ddot{q}_3, q_3 + ha_{21}\dot{q}_4 + ha_{22}\dot{q}_3) \\ & h & f_4(\ddot{q}_4, \dot{q}_3 + ha_{21}\ddot{q}_4 + ha_{22}\ddot{q}_3, q_3 + ha_{21}\dot{q}_4 + ha_{22}\dot{q}_3) \\ \psi_4^T & & S_4\left(\dot{q}_3 + ha_{21}\ddot{q}_4 + ha_{22}\ddot{q}_3 - \dot{q}_4\right) \\ \phi_4^T & & T_4\left(q_3 + ha_{21}\dot{q}_4 + ha_{22}\dot{q}_3 - q_4\right) \end{array}$$

Reverse Mode

We solve for the adjoint variables starting from the last time step.

Step $k = 4$**:**

- Setting $\dfrac{\partial L}{\partial q_4} = 0$, we get:

$$\frac{\partial T_4}{\partial q_4}^T \phi_4 = 0$$

$$\boxed{\phi_4 = 0}$$

- Setting $\dfrac{\partial L}{\partial \dot{q}_4} = 0$, we get:

$$\frac{\partial S_4}{\partial \dot{q}_4}^T \psi_4 + \frac{\partial T_4}{\partial \dot{q}_4}^T \phi_4 = 0$$

$$\boxed{\psi_4 = 0}$$

- Setting $\dfrac{\partial L}{\partial \ddot{q}_4} = 0$, we get:

$$h\frac{\partial R_4}{\partial \ddot{q}_4}^T \lambda_4 + h\frac{\partial f_4}{\partial \ddot{q}_4}^T + \frac{\partial S_4}{\partial \ddot{q}_4}^T \psi_4 = 0$$

$$\boxed{h\left[\frac{\partial R_4}{\partial \ddot{q}_4} + ha_{22}\frac{\partial R_4}{\partial \dot{q}_4} + h^2a_{22}^2\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial \ddot{q}_4} + ha_{22}\frac{\partial f_4}{\partial \dot{q}_4} + h^2a_{22}^2\frac{\partial f_4}{\partial q_4}\right\}^T + ha_{22}\psi_4 = 0}$$

Step $k = 3$**:**

- Setting $\dfrac{\partial L}{\partial q_3} = 0$, we get:

$$\frac{\partial T_3}{\partial q_3}^T \phi_3 + \frac{\partial T_4}{\partial q_3}^T \phi_4 + h\left[\frac{\partial R_4}{\partial q_3}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial q_3}\right\}^T = 0$$

$$\boxed{\phi_3 = \phi_4 + h\left[\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial q_4}\right\}^T}$$

- Setting $\dfrac{\partial L}{\partial \dot{q}_3} = 0$, we get:

$$\frac{\partial S_3}{\partial \dot{q}_3}^T \psi_3 + \frac{\partial T_3}{\partial \dot{q}_3}^T \phi_3 + \frac{\partial S_4}{\partial \dot{q}_3}^T \psi_4 + \frac{\partial T_4}{\partial \dot{q}_3}^T \phi_4 + h\left[\frac{\partial R_4}{\partial \dot{q}_3}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial \dot{q}_3}\right\}^T = 0$$

$$\boxed{\psi_3 = ha_{21}\phi_3 + \psi_4 + ha_{22}\phi_4 + h\left[\frac{\partial R_4}{\partial \dot{q}_4} + ha_{22}\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 + h\left\{\frac{\partial f_4}{\partial \dot{q}_4} + ha_{22}\frac{\partial f_4}{\partial q_4}\right\}^T}$$

- Setting $\dfrac{\partial L}{\partial \ddot{q}_3} = 0$, we get:

$$h\frac{\partial R_3}{\partial \ddot{q}_3}^T \lambda_3 + h\frac{\partial f_3}{\partial \ddot{q}_3}^T + \frac{\partial S_3}{\partial \ddot{q}_3}^T \psi_3 + \frac{\partial T_3}{\partial \ddot{q}_3}^T \phi_3 + \frac{\partial S_4}{\partial \ddot{q}_3}^T \psi_4 + \frac{\partial T_4}{\partial \ddot{q}_3}^T \phi_4 + h\frac{\partial R_4}{\partial \ddot{q}_3}^T \lambda_4 + h\frac{\partial f_4}{\partial \ddot{q}_3}^T = 0$$

$$\begin{aligned} h\left[\frac{\partial R_3}{\partial \ddot{q}_3} + ha_{22}\frac{\partial R_3}{\partial \dot{q}_3} + h^2a_{22}^2\frac{\partial R_3}{\partial q_3}\right]^T \lambda_3 = &- h\left\{\frac{\partial f_3}{\partial \ddot{q}_3} + ha_{22}\frac{\partial f_3}{\partial \dot{q}_3} + h^2a_{22}^2\frac{\partial f_3}{\partial q_3}\right\}^T \\ &- ha_{21}\psi_3 \\ &- h\left[ha_{22}\frac{\partial R_4}{\partial \dot{q}_4} + h^2a_{22}^2\frac{\partial R_4}{\partial q_4}\right]^T \lambda_4 \\ &- h\left\{ha_{22}\frac{\partial f_4}{\partial \dot{q}_4} + h^2a_{22}^2\frac{\partial f_4}{\partial q_4}\right\}^T \\ &- ha_{22}\psi_4 - (ha_{21}ha_{22} + ha_{22}ha_{21})\phi_4 \end{aligned} \tag{1.9}$$

1.4 Diagonally–Implicit–Runge–Kutta

The residual of the governing equations and the objective function of interest are written as follows.

$$R_{ki} = R_{ki}(\ddot{q_{ki}}, \dot{q_{ki}}, q_{ki}, t_{ki}, x)$$

and

$$F_{ki} = hb_i f_{ki}(\ddot{q_{ki}}, \dot{q_{ki}}, q_{ki}, t_{ki}, x).$$

The stage states are,

$$S_k = \dot{q}_{k-1} + h \sum_{i=1}^{s} b_k \ddot{q}_{ki} - \dot{q}_k$$

and

$$T_k = q_{k-1} + h \sum_{i=1}^{s} b_k \dot{q}_{ki} - q_k.$$

$$\mathbf{q_1} \xrightarrow[\dot{q}_{21}, \dot{q}_{22} \cdots \dot{q}_{2s}]{q_{21}, q_{22} \cdots q_{2s}} \mathbf{q_2} \xrightarrow[\dot{q}_{31}, \dot{q}_{32} \cdots \dot{q}_{3s}]{q_{31}, q_{32} \cdots q_{3s}} \mathbf{q_3} \xrightarrow[\dot{q}_{N,1}, \dot{q}_{N,2} \cdots \dot{q}_{N,s}]{q_{N,1}, q_{N,2} \cdots q_{N,s}} \mathbf{q_N}$$

$$\dot{\mathbf{q}}_\mathbf{1} \xrightarrow[\ddot{q}_{21}, \ddot{q}_{22} \cdots \ddot{q}_{2s}]{\dot{q}_{21}, \dot{q}_{22} \cdots \dot{q}_{2s}} \dot{\mathbf{q}}_\mathbf{2} \xrightarrow[\ddot{q}_{31}, \ddot{q}_{32} \cdots \ddot{q}_{3s}]{\dot{q}_{31}, \dot{q}_{32} \cdots \dot{q}_{3s}} \dot{\mathbf{q}}_\mathbf{3} \xrightarrow[\ddot{q}_{N,1}, \ddot{q}_{N,2} \cdots \ddot{q}_{N,s}]{\dot{q}_{N,1}, \dot{q}_{N,2} \cdots \dot{q}_{N,s}} \dot{\mathbf{q}}_\mathbf{N}$$

We form an Lagrangian function:

$$\mathcal{L} = \sum_{k=2}^{N} \sum_{i=1}^{s} hb_i f_{ki} + \sum_{k=2}^{N} \sum_{i=1}^{s} \lambda_{ki}^T hb_i R_{ki} + \sum_{k=1}^{N} \psi_k^T S_k + \sum_{k=1}^{N} \phi_k^T T_k.$$

We find the stationary points of the Lagrangian in an attempt to generate the system of equations to solve for the adjoint variables.

1.4.1 One–Staged DIRK

The one-staged DIRK is a second-order scheme. We write out a few time steps of integration and study the recursive relations.

1.4.2 Two–Staged DIRK

The two-staged DIRK is a third-order scheme. We write out a few time steps of integration and study the recursive relations.

Time step $k = 2$: The state variables have the following relations at this time-step.

$$\begin{aligned}
q_{21} &= q_1 + ha_{11}\dot{q}_{21} \\
q_{22} &= q_1 + ha_{21}\dot{q}_{21} + ha_{22}\dot{q}_{22} \\
\dot{q}_{21} &= \dot{q}_1 + ha_{11}\ddot{q}_{21} \\
\dot{q}_{22} &= \dot{q}_1 + ha_{21}\ddot{q}_{21} + ha_{22}\ddot{q}_{22}
\end{aligned}$$

$$\begin{array}{c|c|l}
\lambda_{21}^T & hb_1 & \mathbf{R_{21}} \left(\underline{\ddot{\mathbf{q}}_\mathbf{21}}, \dot{\mathbf{q}}_\mathbf{21}(\dot{q_1}, \ddot{q_{21}}), \mathbf{q_{21}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}))\right) \\
\lambda_{22}^T & hb_2 & \mathbf{R_{22}} \left(\underline{\ddot{\mathbf{q}}_\mathbf{22}}, \dot{\mathbf{q}}_\mathbf{22}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \mathbf{q_{22}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}))\right) \\
 & hb_1 & \mathbf{f_{21}} \left(\underline{\ddot{\mathbf{q}}_\mathbf{21}}, \dot{\mathbf{q}}_\mathbf{21}(\dot{q_1}, \ddot{q_{21}}), \mathbf{q_{21}}(q_1, \dot{q_{21}}(q_1, \ddot{q_{21}}))\right) \\
 & hb_2 & \mathbf{f_{22}} \left(\underline{\ddot{\mathbf{q}}_\mathbf{22}}, \dot{\mathbf{q}}_\mathbf{22}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \mathbf{q_{22}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}))\right) \\
\psi_2^T & & \mathbf{S_2} \left(\dot{q}_1 + hb_1\ddot{q}_{21} + hb_2\ddot{q}_{22} - \underline{\dot{\mathbf{q}}_\mathbf{2}}\right) \\
\phi_2^T & & \mathbf{T_2} \left(q_1 + hb_1\dot{q}_{21}(\dot{q_1}, \ddot{q_{21}}) + hb_2\dot{q}_{22}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}) - \underline{\mathbf{q_2}}\right)
\end{array}$$

Time Step $k = 3$: The state variables have the following relations at this time-step.

$$
\begin{aligned}
q_{31} &= q_2 + ha_{11}\dot{q}_{31} \\
q_{32} &= q_2 + ha_{21}\dot{q}_{31} + ha_{22}\dot{q}_{32} \\
\dot{q}_{31} &= \dot{q}_2 + ha_{11}\ddot{q}_{31} \\
\dot{q}_{32} &= \dot{q}_2 + ha_{21}\ddot{q}_{31} + ha_{22}\ddot{q}_{32}
\end{aligned}
$$

The equations from this step are:

$$
\begin{array}{l|l|l}
\lambda_{31}^T & hb_1 & \mathbf{R_{31}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{31}}}, \dot{\mathbf{q}}_{\mathbf{31}}(\dot{q_2}, \ddot{q_{31}}), \mathbf{q_{31}}(q_2, \dot{q_{31}}(\dot{q_2}, \ddot{q_{31}}))\right) \\
\lambda_{32}^T & hb_2 & \mathbf{R_{32}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{32}}}, \dot{\mathbf{q}}_{\mathbf{32}}(\dot{q_2}, \ddot{q_{31}}, \ddot{q_{32}}), \mathbf{q_{32}}(q_2, \dot{q_{31}}(\dot{q_2}, \ddot{q_{31}}), \dot{q_{32}}(\dot{q_2}, \ddot{q_{31}}, \ddot{q_{32}}))\right) \\
 & hb_1 & \mathbf{f_{31}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{31}}}, \dot{\mathbf{q}}_{\mathbf{31}}(\dot{q_2}, \ddot{q_{31}}), \mathbf{q_{31}}(q_2, \dot{q_{31}}(\dot{q_2}, \ddot{q_{31}}))\right) \\
 & hb_2 & \mathbf{f_{32}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{32}}}, \dot{\mathbf{q}}_{\mathbf{32}}(\dot{q_2}, \ddot{q_{31}}, \ddot{q_{32}}), \mathbf{q_{32}}(q_2, \dot{q_{31}}(\dot{q_2}, \ddot{q_{31}}), \dot{q_{32}}(\dot{q_2}, \ddot{q_{31}}, \ddot{q_{32}}))\right) \\
\psi_3^T & & \mathbf{S_3}(\dot{q_2} + hb_1\ddot{q}_{31} + hb_2\ddot{q}_{32} - \underline{\dot{\mathbf{q}}_{\mathbf{3}}}) \\
\phi_3^T & & \mathbf{T_3}(q_2 + hb_1\dot{q}_{31}(\dot{q_2}, \ddot{q_{31}}) + hb_2\dot{q}_{32}(\dot{q_2}, \ddot{q_{31}}, \ddot{q_{32}}) - \underline{\mathbf{q_3}})
\end{array}
$$

We operate on these equations and generate the adjoint system of equations.

$$
\begin{array}{l|l}
\dfrac{\partial \mathcal{L}}{\partial q_3} = 0 & \dfrac{\partial T_3}{\partial q_3}^T \phi_3 = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \dot{q}_3} = 0 & \dfrac{\partial S_3}{\partial \dot{q}_3}^T \psi_3 = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_{32}} = 0 & hb_2 \dfrac{\partial R_{32}}{\partial \ddot{q}_{32}}^T \lambda_{32} + \dfrac{\partial T_3}{\partial \ddot{q}_{32}}^T \phi_3 + \dfrac{\partial S_3}{\partial \ddot{q}_{32}}^T \psi_3 + hb_2 \dfrac{\partial f_{32}}{\partial \ddot{q}_{32}}^T = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_{31}} = 0 & hb_1 \dfrac{\partial R_{31}}{\partial \ddot{q}_{31}}^T \lambda_{31} + hb_2 \dfrac{\partial R_{32}}{\partial \ddot{q}_{31}}^T \lambda_{32} + hb_1 \dfrac{\partial f_{31}}{\partial \ddot{q}_{31}}^T + hb_2 \dfrac{\partial f_{32}}{\partial \ddot{q}_{31}}^T + \dfrac{\partial S_3}{\partial \ddot{q}_{31}}^T \psi_3 + \dfrac{\partial T_3}{\partial \ddot{q}_{31}}^T \phi_3 = 0
\end{array}
$$

These equations simplify to the following relations:

$$\phi_3 = 0 \tag{1.10}$$

$$\psi_3 = 0 \tag{1.11}$$

$$
\begin{aligned}
hb_2 \left[\frac{\partial R_{32}}{\partial \ddot{q}_{32}} + ha_{22} \frac{\partial R_{32}}{\partial \dot{q}_{32}} + h^2 a_{22}^2 \frac{\partial R_{32}}{\partial q_{32}} \right]^T \lambda_{32} = &- hb_2 \left[\frac{\partial f_{32}}{\partial \ddot{q}_{32}} + ha_{22} \frac{\partial f_{32}}{\partial \dot{q}_{32}} + h^2 a_{22}^2 \frac{\partial f_{32}}{\partial q_{32}} \right]^T \\
&- hb_2 \psi_3 \\
&- hb_2 ha_{22} \phi_3
\end{aligned} \tag{1.12}
$$

$$
\begin{aligned}
hb_1 \left[\frac{\partial R_{31}}{\partial \ddot{q}_{31}} + ha_{11} \frac{\partial R_{31}}{\partial \dot{q}_{31}} + h^2 a_{11}^2 \frac{\partial R_{31}}{\partial q_{31}} \right]^T \lambda_{31} = &- hb_1 \left[\frac{\partial f_{31}}{\partial \ddot{q}_{31}} + ha_{11} \frac{\partial f_{31}}{\partial \dot{q}_{31}} + h^2 a_{11}^2 \frac{\partial f_{31}}{\partial q_{31}} \right]^T \\
&- hb_2 \left[ha_{21} \frac{\partial f_{32}}{\partial \dot{q}_{32}} + (ha_{21} ha_{11} + ha_{22} ha_{21}) \frac{\partial f_{32}}{\partial q_{32}} \right]^T \\
&- hb_2 \left[ha_{21} \frac{\partial R_{32}}{\partial \dot{q}_{32}} + (ha_{21} ha_{11} + ha_{22} ha_{21}) \frac{\partial R_{32}}{\partial q_{32}} \right]^T \lambda_{32} \\
&- hb_1 \psi_3 \\
&- (hb_1 ha_{11} + hb_2 ha_{21}) \phi_3
\end{aligned} \tag{1.13}
$$

$$\frac{\partial \mathcal{L}}{\partial q_2}=0 \quad \left| \quad \frac{\partial T_2}{\partial q_2}^T\phi_2 + hb_1\frac{\partial R_{31}}{\partial q_2}^T\lambda_{31} + hb_2\frac{\partial R_{32}}{\partial q_2}^T\lambda_{32} + hb_1\frac{\partial f_{31}}{\partial q_2}^T + hb_2\frac{\partial f_{32}}{\partial q_2}^T + \frac{\partial T_3}{\partial q_2}^T\phi_3 = 0\right.$$

$$\frac{\partial \mathcal{L}}{\partial \dot{q}_2}=0 \quad \left| \quad \frac{\partial S_2}{\partial \dot{q}_2}^T\psi_2 + hb_1\frac{\partial R_{31}}{\partial \dot{q}_2}^T\lambda_{31} + hb_2\frac{\partial R_{32}}{\partial \dot{q}_2}^T\lambda_{32} + hb_1\frac{\partial f_{31}}{\partial \dot{q}_2}^T + hb_2\frac{\partial f_{32}}{\partial \dot{q}_2}^T + \frac{\partial T_3}{\partial \dot{q}_2}^T\phi_3 + \frac{\partial S_3}{\partial \dot{q}_2}^T\psi_3 = 0\right.$$

$$\frac{\partial \mathcal{L}}{\partial \ddot{q}_{22}}=0 \quad \left| \quad hb_2\frac{\partial R_{22}}{\partial \ddot{q}_{22}}^T\lambda_{22} + \frac{\partial T_2}{\partial \ddot{q}_{22}}^T\phi_2 + \frac{\partial S_2}{\partial \ddot{q}_{22}}^T\psi_2 + hb_2\frac{\partial f_{22}}{\partial \ddot{q}_{22}}^T = 0\right.$$

$$\frac{\partial \mathcal{L}}{\partial \ddot{q}_{21}}=0 \quad \left| \quad hb_1\frac{\partial R_{21}}{\partial \ddot{q}_{21}}^T\lambda_{21} + hb_2\frac{\partial R_{22}}{\partial \ddot{q}_{21}}^T\lambda_{22} + hb_1\frac{\partial f_{21}}{\partial \ddot{q}_{21}}^T + hb_2\frac{\partial f_{22}}{\partial \ddot{q}_{21}}^T + \frac{\partial S_2}{\partial \ddot{q}_{21}}^T\psi_2 + \frac{\partial T_2}{\partial \ddot{q}_{21}}^T\phi_2 = 0\right.$$

$$\begin{aligned}\psi_2 =& \psi_3 + (hb_1+hb_2)\phi_3 + hb_1\left[\frac{\partial R_{31}}{\partial \dot{q}_{31}} + ha_{11}\frac{\partial R_{31}}{\partial q_{31}}\right]^T\lambda_{31} + hb_1\left[\frac{\partial f_{31}}{\partial \dot{q}_{31}} + ha_{11}\frac{\partial f_{31}}{\partial q_{31}}\right]^T \\ &+ hb_2\left[\frac{\partial R_{32}}{\partial \dot{q}_{32}} + (ha_{21}+ha_{22})\frac{\partial R_{32}}{\partial q_{32}}\right]^T\lambda_{32} + hb_2\left[\frac{\partial f_{32}}{\partial \dot{q}_{32}} + (ha_{21}+ha_{22})\frac{\partial f_{32}}{\partial q_{32}}\right]^T\end{aligned} \tag{1.14}$$

$$\phi_2 = \phi_3 + hb_1\frac{\partial R_{31}}{\partial q_{31}}^T\lambda_{31} + hb_1\frac{\partial f_{31}}{\partial q_{31}}^T + hb_2\frac{\partial R_{32}}{\partial q_{32}}^T\lambda_{32} + hb_2\frac{\partial f_{32}}{\partial q_{32}}^T \tag{1.15}$$

$$\begin{aligned}hb_2\left[\frac{\partial R_{22}}{\partial \ddot{q}_{22}} + ha_{22}\frac{\partial R_{22}}{\partial \dot{q}_{22}} + h^2a_{22}^2\frac{\partial R_{22}}{\partial q_{22}}\right]^T\lambda_{22} =& -hb_2\left[\frac{\partial f_{22}}{\partial \ddot{q}_{22}} + ha_{22}\frac{\partial f_{22}}{\partial \dot{q}_{22}} + h^2a_{22}^2\frac{\partial f_{22}}{\partial q_{22}}\right]^T \\ &- hb_2\psi_2 - hb_2ha_{22}\phi_2\end{aligned} \tag{1.16}$$

$$\begin{aligned}hb_1\left[\frac{\partial R_{21}}{\partial \ddot{q}_{21}} + ha_{11}\frac{\partial R_{21}}{\partial \dot{q}_{21}} + h^2a_{11}^2\frac{\partial R_{21}}{\partial q_{21}}\right]^T\lambda_{21} =& -hb_1\left[\frac{\partial f_{21}}{\partial \ddot{q}_{21}} + ha_{11}\frac{\partial f_{21}}{\partial \dot{q}_{21}} + h^2a_{11}^2\frac{\partial f_{21}}{\partial q_{21}}\right]^T \\ &- hb_2\left[ha_{21}\frac{\partial f_{22}}{\partial \dot{q}_{22}} + (ha_{21}ha_{11}+ha_{22}ha_{21})\frac{\partial f_{22}}{\partial q_{22}}\right]^T \\ &- hb_2\left[ha_{21}\frac{\partial R_{22}}{\partial \dot{q}_{22}} + (ha_{21}ha_{11}+ha_{22}ha_{21})\frac{\partial R_{22}}{\partial q_{22}}\right]^T\lambda_{22} \\ &- hb_1\psi_2 - (hb_1ha_{11}+hb_2ha_{21})\phi_2\end{aligned} \tag{1.17}$$

1.4.3 Three-Staged DIRK

Time step $k = 3$: The state approximations for three-staged DIRK scheme are as follows.

$$\begin{aligned}\dot{q}_{31} &= \dot{q}_2 + ha_{11}\ddot{q}_{31} \\ \dot{q}_{32} &= \dot{q}_2 + ha_{21}\ddot{q}_{31} + ha_{22}\ddot{q}_{32} \\ \dot{q}_{33} &= \dot{q}_2 + ha_{31}\ddot{q}_{31} + ha_{32}\ddot{q}_{32} + ha_{33}\ddot{q}_{33}\end{aligned}$$

$$\begin{aligned}q_{31} &= q_2 + ha_{11}\dot{q}_{31} \\ q_{32} &= q_2 + ha_{21}\dot{q}_{31} + ha_{22}\dot{q}_{32} \\ q_{33} &= q_2 + ha_{31}\dot{q}_{31} + ha_{32}\dot{q}_{32} + ha_{33}\dot{q}_{33}\end{aligned}$$

$$
\begin{array}{c|c|l}
\lambda_{31}^T & hb_1 & \mathbf{R_{31}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{31}}}, \dot{\mathbf{q}}_{\mathbf{31}}(\dot q_2, \ddot q_{31}), \mathbf{q_{31}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}))\right) \\
\lambda_{32}^T & hb_2 & \mathbf{R_{32}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{32}}}, \dot{\mathbf{q}}_{\mathbf{32}}(\dot q_2, \ddot q_{31}, \ddot q_{32}), \mathbf{q_{32}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}), \dot q_{32}(\dot q_2, \ddot q_{31}, \ddot q_{32}))\right) \\
\lambda_{33}^T & hb_3 & \mathbf{R_{33}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{33}}}, \dot{\mathbf{q}}_{\mathbf{33}}(\dot q_2, \ddot q_{31}, \ddot q_{32}, \ddot q_{33}), \mathbf{q_{33}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}), \dot q_{32}(\dot q_2, \ddot q_{31}, \ddot q_{32}), \dot q_{33}(\dot q_2, \ddot q_{31}, \ddot q_{32}, \ddot q_{33}))\right) \\
 & hb_1 & \mathbf{f_{31}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{31}}}, \dot{\mathbf{q}}_{\mathbf{31}}(\dot q_2, \ddot q_{31}), \mathbf{q_{31}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}))\right) \\
 & hb_2 & \mathbf{f_{32}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{32}}}, \dot{\mathbf{q}}_{\mathbf{32}}(\dot q_2, \ddot q_{31}, \ddot q_{32}), \mathbf{q_{32}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}), \dot q_{32}(\dot q_2, \ddot q_{31}, \ddot q_{32}))\right) \\
 & hb_3 & \mathbf{f_{33}}\left(\underline{\ddot{\mathbf{q}}_{\mathbf{33}}}, \dot{\mathbf{q}}_{\mathbf{33}}(\dot q_2, \ddot q_{31}, \ddot q_{33}, \ddot q_{33}), \mathbf{q_{32}}(q_2, \dot q_{31}(\dot q_2, \ddot q_{31}), \dot q_{32}(\dot q_2, \ddot q_{31}, \ddot q_{32}), \dot q_{33}(\dot q_2, \ddot q_{31}, \ddot q_{32}, \ddot q_{33}))\right) \\
\phi_3^T & & \mathbf{T_3}(q_2 + hb_1\dot q_{31}(\dot q_2, \ddot q_{31}) + hb_2\dot q_{32}(\dot q_2, \ddot q_{31}, \ddot q_{32}) + hb_3\dot q_{33}(\dot q_2, \ddot q_{31}, \ddot q_{32}, \ddot q_{33}) - \underline{\mathbf{q_3}}) \\
\psi_3^T & & \mathbf{S_3}(\dot q_2 + hb_1\ddot q_{31} + hb_2\ddot q_{32} + hb_3\ddot q_{33} - \underline{\dot{\mathbf{q}}_{\mathbf{3}}})
\end{array}
$$

The adjoint variables at this step are $\psi_3, \phi_3, \lambda_{31}, \lambda_{32}, \lambda_{33}$.

$$
\begin{array}{l|l}
\dfrac{\partial \mathcal{L}}{\partial q_3} = 0 & \dfrac{\partial T_3}{\partial q_3}^T \phi_3 = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \dot q_3} = 0 & \dfrac{\partial S_3}{\partial \dot q_3}^T \psi_3 = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \ddot q_{33}} = 0 & hb_3 \dfrac{\partial R_{33}}{\partial \ddot q_{33}}^T \lambda_{33} + \dfrac{\partial T_3}{\partial \ddot q_{33}}^T \phi_3 + \dfrac{\partial S_3}{\partial \ddot q_{33}}^T \psi_3 + hb_3 \dfrac{\partial f_{33}}{\partial \ddot q_{33}}^T = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \ddot q_{32}} = 0 & hb_2 \dfrac{\partial R_{32}}{\partial \ddot q_{32}}^T \lambda_{32} + hb_3 \dfrac{\partial R_{33}}{\partial \ddot q_{32}}^T \lambda_{33} + \dfrac{\partial T_3}{\partial \ddot q_{32}}^T \phi_3 + \dfrac{\partial S_3}{\partial \ddot q_{32}}^T \psi_3 + hb_2 \dfrac{\partial f_{32}}{\partial \ddot q_{32}}^T + + hb_3 \dfrac{\partial f_{33}}{\partial \ddot q_{32}}^T = 0 \\[2ex]
\dfrac{\partial \mathcal{L}}{\partial \ddot q_{31}} = 0 & hb_1 \dfrac{\partial R_{31}}{\partial \ddot q_{31}}^T \lambda_{31} + hb_2 \dfrac{\partial R_{32}}{\partial \ddot q_{31}}^T \lambda_{32} + hb_3 \dfrac{\partial R_{33}}{\partial \ddot q_{31}}^T \lambda_{33} + \dfrac{\partial S_3}{\partial \ddot q_{31}}^T \psi_3 + \dfrac{\partial T_3}{\partial \ddot q_{31}}^T \phi_3 + \\
 & hb_1 \dfrac{\partial f_{31}}{\partial \ddot q_{31}}^T + hb_2 \dfrac{\partial f_{32}}{\partial \ddot q_{31}}^T + hb_3 \dfrac{\partial f_{33}}{\partial \ddot q_{31}}^T = 0
\end{array}
$$

$$\phi_3 = 0 \tag{1.18}$$

$$\psi_3 = 0 \tag{1.19}$$

$$
\begin{aligned}
hb_3 \left[\frac{\partial R_{33}}{\partial \ddot q_{33}} + ha_{33}\frac{\partial R_{33}}{\partial \dot q_{33}} + h^2 a_{33}^2 \frac{\partial R_{33}}{\partial q_{33}}\right]^T \lambda_{33} = & - hb_3 \left[\frac{\partial f_{33}}{\partial \ddot q_{33}} + ha_{33}\frac{\partial f_{33}}{\partial \dot q_{33}} + h^2 a_{33}^2 \frac{\partial f_{33}}{\partial q_{33}}\right]^T \\
& - hb_3\psi_3 \\
& - hb_3 ha_{33}\phi_3
\end{aligned} \tag{1.20}
$$

$$
\begin{aligned}
hb_2 \left[\frac{\partial R_{32}}{\partial \ddot q_{32}} + ha_{22}\frac{\partial R_{32}}{\partial \dot q_{32}} + h^2 a_{22}^2 \frac{\partial R_{32}}{\partial q_{32}}\right]^T \lambda_{32} = & - hb_2 \left[\frac{\partial f_{32}}{\partial \ddot q_{32}} + ha_{22}\frac{\partial f_{32}}{\partial \dot q_{32}} + h^2 a_{22}^2 \frac{\partial f_{32}}{\partial q_{32}}\right]^T \\
& - hb_3 \left[ha_{32}\frac{\partial f_{33}}{\partial \dot q_{33}} + (ha_{32}ha_{22} + ha_{33}ha_{32})\frac{\partial f_{33}}{\partial q_{33}}\right]^T \\
& - hb_3 \left[ha_{32}\frac{\partial R_{33}}{\partial \dot q_{33}} + (ha_{32}ha_{22} + ha_{33}ha_{32})\frac{\partial R_{33}}{\partial q_{33}}\right]^T \lambda_{33} \\
& - hb_2\psi_3 \\
& - (hb_2 ha_{22} + hb_3 ha_{32})\phi_3
\end{aligned} \tag{1.21}
$$

$$
\begin{aligned}
hb_1 \left[\frac{\partial R_{31}}{\partial \ddot{q}_{31}} + ha_{11} \frac{\partial R_{31}}{\partial \dot{q}_{31}} + h^2 a_{11}^2 \frac{\partial R_{31}}{\partial q_{31}} \right]^T \lambda_{31} = & - hb_1 \left[\frac{\partial f_{31}}{\partial \ddot{q}_{31}} + ha_{11} \frac{\partial f_{31}}{\partial \dot{q}_{31}} + h^2 a_{11}^2 \frac{\partial f_{31}}{\partial q_{31}} \right]^T \\
& - hb_2 \left[ha_{21} \frac{\partial R_{32}}{\partial \dot{q}_{32}} + (ha_{21} ha_{11} + ha_{22} ha_{21}) \frac{\partial R_{32}}{\partial q_{32}} \right] \lambda_{32} \\
& - hb_2 \left[ha_{21} \frac{\partial f_{32}}{\partial \dot{q}_{32}} + (ha_{21} ha_{11} + ha_{22} ha_{21}) \frac{\partial f_{32}}{\partial q_{32}} \right] \\
& - hb_3 \left[ha_{31} \frac{\partial R_{33}}{\partial \dot{q}_{33}} + (ha_{31} ha_{11} + ha_{32} ha_{21} + ha_{33} ha_{31}) \frac{\partial R_{33}}{\partial q_{33}} \right] \lambda_{33} \\
& - hb_3 \left[ha_{31} \frac{\partial f_{33}}{\partial \dot{q}_{33}} + (ha_{31} ha_{11} + ha_{32} ha_{21} + ha_{33} ha_{31}) \frac{\partial f_{33}}{\partial q_{33}} \right] \\
& - hb_1 \psi_3 \\
& - (hb_1 ha_{11} + hb_2 ha_{21} + hb_3 ha_{31}) \phi_3
\end{aligned}
\tag{1.22}
$$

Time step $k = 2$: The state approximations at this step are as follows.

$$
\begin{aligned}
\dot{q}_{21} &= \dot{q}_1 + ha_{11} \ddot{q}_{21} \\
\dot{q}_{22} &= \dot{q}_1 + ha_{21} \ddot{q}_{21} + ha_{22} \ddot{q}_{22} \\
\dot{q}_{23} &= \dot{q}_1 + ha_{31} \ddot{q}_{21} + ha_{32} \ddot{q}_{22} + ha_{33} \ddot{q}_{23}
\end{aligned}
$$

$$
\begin{aligned}
q_{21} &= q_1 + ha_{11} \dot{q}_{21} \\
q_{22} &= q_1 + ha_{21} \dot{q}_{21} + ha_{22} \dot{q}_{22} \\
q_{23} &= q_1 + ha_{31} \dot{q}_{21} + ha_{32} \dot{q}_{22} + ha_{33} \dot{q}_{23}
\end{aligned}
$$

The equations and the associated adjoint variables are shown here.

$$
\begin{array}{c|c|l}
\lambda_{21}^T & hb_1 & \mathbf{R_{21}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{21}}}, \dot{\mathbf{q}}_{\mathbf{21}}(\dot{q_1}, \ddot{q_{21}}), \mathbf{q_{21}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}})) \right) \\
\lambda_{22}^T & hb_2 & \mathbf{R_{22}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{22}}}, \dot{\mathbf{q}}_{\mathbf{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \mathbf{q_{22}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}})) \right) \\
\lambda_{23}^T & hb_3 & \mathbf{R_{23}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{23}}}, \dot{\mathbf{q}}_{\mathbf{23}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}, \ddot{q_{23}}), \mathbf{q_{23}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \dot{q_{23}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}, \ddot{q_{23}})) \right) \\
 & hb_1 & \mathbf{f_{21}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{21}}}, \dot{\mathbf{q}}_{\mathbf{21}}(\dot{q_1}, \ddot{q_{21}}), \mathbf{q_{21}}(q_1, \dot{q_{21}}(q_1, \ddot{q_{21}})) \right) \\
 & hb_2 & \mathbf{f_{22}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{22}}}, \dot{\mathbf{q}}_{\mathbf{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \mathbf{q_{22}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}})) \right) \\
 & hb_3 & \mathbf{f_{23}} \left(\underline{\ddot{\mathbf{q}}_{\mathbf{23}}}, \dot{\mathbf{q}}_{\mathbf{23}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}, \ddot{q_{23}}), \mathbf{q_{23}}(q_1, \dot{q_{21}}(\dot{q_1}, \ddot{q_{21}}), \dot{q_{22}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}), \dot{q_{23}}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}, \ddot{q_{23}})) \right) \\
\psi_2^T & & \mathbf{S_2} \left(\dot{q}_1 + hb_1 \ddot{q}_{21} + hb_2 \ddot{q}_{22} + hb_2 \ddot{q}_{23} - \underline{\dot{\mathbf{q}}_{\mathbf{2}}} \right) \\
\phi_2^T & & \mathbf{T_2} \left(q_1 + hb_1 \dot{q}_{21}(\dot{q_1}, \ddot{q_{21}}) + hb_2 \dot{q}_{22}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}) + hb_3 \dot{q}_{23}(\dot{q_1}, \ddot{q_{21}}, \ddot{q_{22}}, \ddot{q_{23}}) - \underline{\mathbf{q_2}} \right)
\end{array}
$$

The adjoint variables at this time step are $\psi_2, \phi_2, \lambda_{31}, \lambda_{32}, \lambda_{33}$.

$$
\begin{array}{l|l}
\dfrac{\partial \mathcal{L}}{\partial q_2} = 0 & \dfrac{\partial T_2}{\partial q_2}^T \phi_2 + hb_1 \dfrac{\partial R_{31}}{\partial q_2}^T \lambda_{31} + hb_2 \dfrac{\partial R_{32}}{\partial q_2}^T \lambda_{32} + hb_3 \dfrac{\partial R_{33}}{\partial q_2}^T \lambda_{33} \\
& +hb_1 \dfrac{\partial f_{31}}{\partial q_2}^T + hb_2 \dfrac{\partial f_{32}}{\partial q_2}^T + hb_3 \dfrac{\partial f_{33}}{\partial q_2}^T + \dfrac{\partial T_3}{\partial q_2}^T \phi_3 = 0 \\
& \\
\dfrac{\partial \mathcal{L}}{\partial \dot{q}_2} = 0 & \dfrac{\partial S_2}{\partial \dot{q}_2}^T \psi_2 + hb_1 \dfrac{\partial R_{31}}{\partial \dot{q}_2}^T \lambda_{31} + hb_2 \dfrac{\partial R_{32}}{\partial \dot{q}_2}^T \lambda_{32} + hb_3 \dfrac{\partial R_{33}}{\partial \dot{q}_2}^T \lambda_{33} \\
& +hb_1 \dfrac{\partial f_{31}}{\partial \dot{q}_2}^T + hb_2 \dfrac{\partial f_{32}}{\partial \dot{q}_2}^T + hb_3 \dfrac{\partial f_{33}}{\partial \dot{q}_2}^T + \dfrac{\partial T_3}{\partial \dot{q}_2}^T \phi_3 + \dfrac{\partial S_3}{\partial \dot{q}_2}^T \psi_3 = 0 \\
& \\
\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_{23}} = 0 & hb_3 \dfrac{\partial R_{23}}{\partial \ddot{q}_{23}}^T \lambda_{23} + \dfrac{\partial T_2}{\partial \ddot{q}_{23}}^T \phi_2 + \dfrac{\partial S_2}{\partial \ddot{q}_{23}}^T \psi_2 + hb_3 \dfrac{\partial f_{23}}{\partial \ddot{q}_{23}}^T = 0 \\
& \\
\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_{22}} = 0 & hb_2 \dfrac{\partial R_{22}}{\partial \ddot{q}_{22}}^T \lambda_{22} + hb_3 \dfrac{\partial R_{23}}{\partial \ddot{q}_{22}}^T \lambda_{23} + \dfrac{\partial T_3}{\partial \ddot{q}_{22}}^T \phi_3 + \dfrac{\partial S_3}{\partial \ddot{q}_{22}}^T \psi_3 + hb_2 \dfrac{\partial f_{22}}{\partial \ddot{q}_{22}}^T + +hb_3 \dfrac{\partial f_{23}}{\partial \ddot{q}_{22}}^T = 0 \\
& \\
\dfrac{\partial \mathcal{L}}{\partial \ddot{q}_{21}} = 0 & hb_1 \dfrac{\partial R_{21}}{\partial \ddot{q}_{21}}^T \lambda_{21} + hb_2 \dfrac{\partial R_{22}}{\partial \ddot{q}_{21}}^T \lambda_{22} + hb_3 \dfrac{\partial R_{23}}{\partial \ddot{q}_{21}}^T \lambda_{23} + \dfrac{\partial S_3}{\partial \ddot{q}_{21}}^T \psi_3 + \dfrac{\partial T_3}{\partial \ddot{q}_{21}}^T \phi_3 + \\
& hb_1 \dfrac{\partial f_{21}}{\partial \ddot{q}_{21}}^T + hb_2 \dfrac{\partial f_{22}}{\partial \ddot{q}_{21}}^T + hb_3 \dfrac{\partial f_{23}}{\partial \ddot{q}_{21}}^T = 0
\end{array}
$$

$$
\phi_2 = \phi_3 + hb_1 \frac{\partial R_{31}}{\partial q_{31}}^T \lambda_{31} + hb_1 \frac{\partial f_{31}}{\partial q_{31}}^T + hb_2 \frac{\partial R_{32}}{\partial q_{32}}^T \lambda_{32} + hb_2 \frac{\partial f_{32}}{\partial q_{32}}^T + hb_3 \frac{\partial R_{33}}{\partial q_{33}}^T \lambda_{33} + hb_3 \frac{\partial f_{33}}{\partial q_{33}}^T \tag{1.23}
$$

$$
\begin{aligned}
\psi_2 = & \psi_3 + (hb_1 + hb_2 + hb_3)\phi_3 \\
& + hb_1 \left[\frac{\partial R_{31}}{\partial \dot{q}_{31}} + ha_{11} \frac{\partial R_{31}}{\partial q_{31}} \right]^T \lambda_{31} + hb_1 \left[\frac{\partial f_{31}}{\partial \dot{q}_{31}} + ha_{11} \frac{\partial f_{31}}{\partial q_{31}} \right]^T \\
& + hb_2 \left[\frac{\partial R_{32}}{\partial \dot{q}_{32}} + (ha_{21} + ha_{22}) \frac{\partial R_{32}}{\partial q_{32}} \right]^T \lambda_{32} + hb_2 \left[\frac{\partial f_{32}}{\partial \dot{q}_{32}} + (ha_{21} + ha_{22}) \frac{\partial f_{32}}{\partial q_{32}} \right]^T \\
& + hb_3 \left[\frac{\partial R_{33}}{\partial \dot{q}_{33}} + (ha_{31} + ha_{32} + ha_{33}) \frac{\partial R_{33}}{\partial q_{33}} \right]^T \lambda_{33} + hb_3 \left[\frac{\partial f_{33}}{\partial \dot{q}_{33}} + (ha_{31} + ha_{32} + ha_{33}) \frac{\partial f_{33}}{\partial q_{33}} \right]^T
\end{aligned} \tag{1.24}
$$

$$
\begin{aligned}
hb_3 \left[\frac{\partial R_{23}}{\partial \ddot{q}_{23}} + ha_{33} \frac{\partial R_{23}}{\partial \dot{q}_{23}} + h^2 a_{33}^2 \frac{\partial R_{23}}{\partial q_{23}} \right]^T \lambda_{23} = & - hb_3 \left[\frac{\partial f_{23}}{\partial \ddot{q}_{23}} + ha_{33} \frac{\partial f_{23}}{\partial \dot{q}_{23}} + h^2 a_{33}^2 \frac{\partial f_{23}}{\partial q_{23}} \right]^T \\
& - hb_3 \psi_2 \\
& - hb_3 ha_{33} \phi_2
\end{aligned} \tag{1.25}
$$

$$
\begin{aligned}
hb_2 \left[\frac{\partial R_{22}}{\partial \ddot{q}_{22}} + ha_{22} \frac{\partial R_{22}}{\partial \dot{q}_{22}} + h^2 a_{22}^2 \frac{\partial R_{22}}{\partial q_{22}} \right]^T \lambda_{22} = & - hb_2 \left[\frac{\partial f_{22}}{\partial \ddot{q}_{22}} + ha_{22} \frac{\partial f_{22}}{\partial \dot{q}_{22}} + h^2 a_{22}^2 \frac{\partial f_{22}}{\partial q_{22}} \right]^T \\
& - hb_3 \left[ha_{32} \frac{\partial f_{23}}{\partial \dot{q}_{23}} + (ha_{32} ha_{22} + ha_{33} ha_{32}) \frac{\partial f_{23}}{\partial q_{23}} \right]^T \\
& - hb_3 \left[ha_{32} \frac{\partial R_{23}}{\partial \dot{q}_{23}} + (ha_{32} ha_{22} + ha_{33} ha_{32}) \frac{\partial R_{23}}{\partial q_{23}} \right]^T \lambda_{23} \\
& - hb_2 \psi_2 \\
& - (hb_2 ha_{22} + hb_3 ha_{32}) \phi_2
\end{aligned} \tag{1.26}
$$

$$\begin{aligned}
hb_1\left[\frac{\partial R_{21}}{\partial \ddot{q}_{21}} + ha_{11}\frac{\partial R_{21}}{\partial \dot{q}_{21}} + h^2a_{11}^2\frac{\partial R_{21}}{\partial q_{21}}\right]^T\lambda_{21} = &- hb_1\left[\frac{\partial f_{21}}{\partial \ddot{q}_{21}} + ha_{11}\frac{\partial f_{21}}{\partial \dot{q}_{21}} + h^2a_{11}^2\frac{\partial f_{21}}{\partial q_{21}}\right]^T \\
&- hb_2\left[ha_{21}\frac{\partial R_{22}}{\partial \dot{q}_{22}} + (ha_{21}ha_{11} + ha_{22}ha_{21})\frac{\partial R_{22}}{\partial q_{22}}\right]\lambda_{22} \\
&- hb_2\left[ha_{21}\frac{\partial f_{22}}{\partial \dot{q}_{22}} + (ha_{21}ha_{11} + ha_{22}ha_{21})\frac{\partial f_{22}}{\partial q_{22}}\right] \\
&- hb_3\left[ha_{31}\frac{\partial R_{23}}{\partial \dot{q}_{23}} + (ha_{31}ha_{11} + ha_{32}ha_{21} + ha_{33}ha_{31})\frac{\partial R_{23}}{\partial q_{23}}\right]\lambda_{23} \\
&- hb_3\left[ha_{31}\frac{\partial f_{23}}{\partial \dot{q}_{23}} + (ha_{31}ha_{11} + ha_{32}ha_{21} + ha_{33}ha_{31})\frac{\partial f_{23}}{\partial q_{23}}\right] \\
&- hb_1\psi_2 \\
&- (hb_1ha_{11} + hb_2ha_{21} + hb_3ha_{31})\phi_2
\end{aligned} \tag{1.27}$$

General DIRK Adjoint Relations: We introduce λ, ϕ and ψ as adjoint variables associated with equations R, T and S. The Lagrangian is

$$\mathcal{L} = \sum_{k=2}^{N}\sum_{i=1}^{s} hb_i f_{ki} + \sum_{k=2}^{N}\sum_{i=1}^{s}\lambda_{ki}^T hb_i R_{ki} + \sum_{k=1}^{N}\phi_k^T T_k + \sum_{k=1}^{N}\psi_k^T S_k.$$

Position adjoint:

$$\phi_k = \phi_{k+1} + h\sum_{i=1}^{s} b_i\left[\frac{\partial R_{k+1,i}}{\partial q_{k+1,i}}\right]^T\lambda_{k+1,i} + h\sum_{i=1}^{s} b_i\left[\frac{\partial f_{k+1,i}}{\partial q_{k+1,i}}\right]^T$$

Here,

$$\alpha = hb_i, \beta = 0, \gamma = 0$$

Velocity adjoint:

$$\begin{aligned}
\psi_k = \psi_{k+1} + \left(h\sum_{i=1}^{s} b_i\right)\phi_{k+1} &+ h\sum_{i=1}^{s} b_i\left[\frac{\partial R_{k+1,i}}{\partial \dot{q}_{k+1,i}} + \left(h\sum_{j=1}^{i} a_{ij}\right)\frac{\partial R_{k+1,i}}{\partial q_{k+1,i}}\right]^T\lambda_{k+1,i} \\
&+ h\sum_{i=1}^{s} b_i\left[\frac{\partial f_{k+1,i}}{\partial \dot{q}_{k+1,i}} + \left(h\sum_{j=1}^{i} a_{ij}\right)\frac{\partial f_{k+1,i}}{\partial q_{k+1,i}}\right]^T
\end{aligned}$$

Noting that $\sum_{i=1}^{s} b_i = 1$, and $\sum_{j=1}^{i} a_{ij} = c_i$,

$$\begin{aligned}
\psi_k = \psi_{k+1} + h\phi_{k+1} &+ h\sum_{i=1}^{s} b_i\left[\frac{\partial R_{k+1,i}}{\partial \dot{q}_{k+1,i}} + hc_i\frac{\partial R_{k+1,i}}{\partial q_{k+1,i}}\right]^T\lambda_{k+1,i} \\
&+ h\sum_{i=1}^{s} b_i\left[\frac{\partial f_{k+1,i}}{\partial \dot{q}_{k+1,i}} + hc_i\frac{\partial f_{k+1,i}}{\partial q_{k+1,i}}\right]^T
\end{aligned}$$

Therefore

$$\beta = hb_i, \alpha = \beta hc_i, \gamma = 0.$$

Primary adjoint: Taking $\partial \mathcal{L}/\partial \ddot{q}_{ki} = 0$ yields

$$
\begin{aligned}
0 = hb_i \frac{\partial f_{ki}}{\partial \ddot{q}_{ki}} &+ \sum_{j=i}^{s} b_j \left[ha_{ji} \frac{\partial f_{kj}}{\partial \dot{q}_{kj}} + h^2 (\sum_{p=i}^{j} a_{jp} a_{pi}) \frac{\partial f_{kj}}{\partial q_{kj}} \right]^T \\
+ hb_i \frac{\partial R_{ki}}{\partial \ddot{q}_{ki}} &+ \sum_{j=i}^{s} b_j \left[ha_{ji} \frac{\partial R_{kj}}{\partial \dot{q}_{kj}} + h^2 (\sum_{p=i}^{j} a_{jp} a_{pi}) \frac{\partial R_{kj}}{\partial q_{kj}} \right]^T \lambda_{kj} \\
+ \sum_{j=i}^{s} hb_j ha_{ji} \phi_k & \\
+ hb_i \psi_k &
\end{aligned}
$$

Note the similarities in the terms arising from the governing equation and the function.

$$
\begin{aligned}
b_i \left[\frac{\partial R_{ki}}{\partial \ddot{q}_{ki}} + ha_{ii} \frac{\partial R_{ki}}{\partial \dot{q}_{ki}} + h^2 a_{ii}^2 \frac{\partial R_{ki}}{\partial q_{ki}} \right]^T \lambda_{ki} = &- b_i \left[\frac{\partial f_{ki}}{\partial \ddot{q}_{ki}} + h^2 a_{ii}^2 \frac{\partial f_{ki}}{\partial \dot{q}_{ki}} + h^2 a_{ii}^2 \frac{\partial f_{ki}}{\partial q_{ki}} \right]^T \\
&- \sum_{j=i+1}^{s} b_j \left[ha_{ji} \frac{\partial R_{kj}}{\partial \dot{q}_{kj}} + h^2 (\sum_{p=i}^{j} a_{jp} a_{pi}) \frac{\partial R_{kj}}{\partial q_{kj}} \right]^T \lambda_{kj} \\
&- \sum_{j=i+1}^{s} b_j \left[ha_{ji} \frac{\partial f_{kj}}{\partial \dot{q}_{kj}} + h^2 (\sum_{p=i}^{j} a_{jp} a_{pi}) \frac{\partial f_{kj}}{\partial q_{kj}} \right]^T \\
&- (\sum_{j=i}^{s} hb_j a_{ji}) \phi_k \\
&- b_i \psi_k
\end{aligned}
$$