Efficient Computation of Higher-Order Variational Integrators in Robotic Simulation and Trajectory Optimization: Appendix

Taosha Fan   Jarvis Shultz   Todd Murphey

Department of Mechanical Engineering, Northwestern University,
2145 Sheridan Road, Evanston, IL 60208, USA
taosha.fan@u.northwestern.edu, jschultz@northwestern.edu,
t-murphey@northwestern.edu

Abstract. This appendix provides the complete $O(n)$ algorithms to compute the Newton direction for higher-order variational integrators and the proofs of the propositions in the paper "Efficient Computation of Higher-Order Variational Integrators in Robotic Simulation and Trajectory Optimization" [1], accepted to the 13th International Workshop on the Algorithmic Foundations of Robotics (WAFR'18). It is assumed that the reader has read the original paper and knows the problem statements and the notation used. The numbering of the equations, algorithms, propositions, etc., is consistent with the numbering used in the original paper.

A Introduction

In the paper "Efficient Computation of Higher-Order Variational Integrators in Robotic Simulation and Trajectory Optimization" [1], we present $O(n)$ algorithms to evaluate the discrete Euler-Lagrange (DEL) equations and compute the Newton direction for solving the DEL equations, and $O(n^2)$ algorithms to linearize the DEL equations. As an appendix to [1], this document provides the complete $O(n)$ algorithms to compute the Newton direction for higher-order variational integrators and the proofs of the propositions in [1], which are not covered in the original paper due to space limitations.

In this appendix, we begin with the complete $O(n)$ algorithms to compute the Newton direction in Section B. In Section C, we give an overview of preliminaries used in the algorithms and proofs. Propositions 1 to 4 in [1, Sections 3 and 4] to compute the higher-order variational integrators are proved in Section D.

For implementation only, the reader only needs to read Algorithms B.1 and B.2 in Section B as well as Algorithms 1 to 3 in [1, Sections 3 and 4]. Sections C and D are not required to read as they present the proofs of the propositions in [1] that do not necessarily aid in implementation.

Even though most of the important content in [1] is reiterated, we still advise the reader to read the original paper to know the problem statements and the notation used. Moreover, as mentioned in the abstract, the numbering of the equations, algorithms, propositions, etc., is consistent with the numbering used in [1]. Therefore, the original paper will not be explicitly cited in the rest of this appendix when we make references to anything in it.

B The $O(n)$ Algorithms to Compute the Newton Direction

In this section, we present Algorithms B.1 and B.2 to compute the Newton direction for higher-order variational integrators. The algorithms are self-contained and we refer the reader to Section C.3 for differentiation on Lie groups that is used to compute $\mathbb{D}_1\overline{F}_i^{k,\alpha}$ in Eq. (B.3b) of Algorithm B.2. The correctness and the $O(n)$ complexity of Algorithms B.1 and B.2 are proved in Section D.2, however, this is not required to read for implementation. We remind the reader that $\delta q_i^{k,\gamma}$ is the Newton direction for $q_i^{k,\gamma}$, and $r_i^{k,\varrho}$ is the residue of the DEL equations Eqs. (7a) and (7b). Moreover, from Proposition 2, Algorithms B.1 and B.2 assume that the inverse of the Jacobian $\mathcal{J}^{-1}(\overline{q}^k)$ exists, and $\overline{F}_i^{k,\alpha}$ and $Q_i^{k,\alpha}$ can be respectively formulated as $\overline{F}_i^{k,\alpha} = \overline{F}_i^{k,\alpha}(g_i^{k,\alpha}, \overline{v}_i^{k,\alpha}, u^{k,\alpha})$ and $Q_i^{k,\alpha} = Q_i^{k,\alpha}(q_i^{k,\alpha}, \dot{q}_i^{k,\alpha}, u^{k,\alpha})$.

There are a number of quantities, such as $D_i^{k,\alpha\rho}$, $\Phi_i^{k,\alpha\gamma}$, $\zeta_i^{k,\alpha}$, $H_i^{k,\gamma}$, etc., which are recursively introduced in Algorithm B.2 to compute the Newton direction. Since there is no influence on the implementation of the algorithms as long as these quantities are correctly computed, we leave the explanation of their meaning to Section D.2. Similarly, the detailed explanation of $\overline{\eta}_i^{k,\nu}$ and $\overline{\delta}\overline{v}_i^{k,\rho}$ in Algorithm B.1 is left to Sections C.1 and C.2, respectively. For purposes of implementation, the reader only needs to know that these quantities are recursively computed through Algorithms B.1 and B.2.

Algorithm B.1 Recursive Computation of the Newton Direction

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initialize $g_0^{k,\alpha} = \mathbf{I}$ and $\overline{v}_0^{k,\alpha} = 0$
for $i = 1 \to n$ **do**
    for $\alpha = 0 \to s$ **do**
        $g_i^{k,\alpha} = g_{\mathrm{par}(i)}^{k,\alpha} g_{\mathrm{par}(i),i}^{k,\alpha}(q_i^{k,\alpha})$
        $\overline{S}_i^{k,\alpha} = \mathrm{Ad}_{g_i^{k,\alpha}} S_i, \quad \overline{M}_i^{k,\alpha} = \mathrm{Ad}_{g_i^{k,\alpha}}^{-T} M_i \mathrm{Ad}_{g_i^{k,\alpha}}^{-1}$
        $\dot{q}_i^{k,\alpha} = \frac{1}{\Delta t}\sum\limits_{\beta=0}^{s} b^{\alpha\beta} q_i^{k,\beta}, \quad \overline{v}_i^{k,\alpha} = \overline{v}_{\mathrm{par}(i)}^{k,\alpha} + \overline{S}_i^{k,\alpha} \cdot \dot{q}_i^{k,\alpha}$
        $\dot{\overline{S}}_i^{k,\alpha} = \mathrm{ad}_{\overline{v}_i^{k,\alpha}} \overline{S}_i^{k,\alpha}$
    end for
end for
for $i = n \to 1$ **do**
    use Algorithm B.2 to evaluate
        a) $D_i^{k,\alpha\rho}$, $G_i^{k,\alpha\nu}$, $l_i^{k,\alpha}$ and $\overline{\mu}_i^{k,\alpha}$
        b) $\Pi_i^{k,\alpha\rho}$, $\Psi_i^{k,\alpha\nu}$, $\zeta_i^{k,\alpha}$ and $\overline{\Gamma}_i^{k,\alpha}$
        c) $H_i^{k,\alpha}$ and $\Phi_i^{k,\alpha}$
        d) $X_i^{k,\alpha\rho}$, $Y_i^{k,\alpha\nu}$ and $y_i^{k,\alpha}$
end for
initialize $\overline{\eta}_0^{k,\nu} = 0$ and $\overline{\delta}\overline{v}_0^{k,\rho} = 0$
for $i = 1 \to n$ **do**

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        for γ = 1 → s do
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$$\delta q_i^{k,\gamma} = \sum_{\rho=0}^{s} X_i^{k,\gamma\rho} \cdot \overline{\delta v}_{\mathrm{par}(i)}^{k,\rho} + \sum_{\nu=1}^{s} Y_i^{k,\gamma\nu} \cdot \overline{\eta}_{\mathrm{par}(i)}^{k,\nu} + y_i^{k,\gamma}$$

end for

for $\nu = 1 \to s$ **do**

$$\overline{\eta}_i^{k,\nu} = \overline{\eta}_{\mathrm{par}(i)}^{k,\nu} + \overline{S}_i^{k,\nu} \cdot \delta q_i^{k,\nu}$$

end for

for $\rho = 0 \to s$ **do**

$$\delta \dot{q}_i^{k,\rho} = \frac{1}{\Delta t} \sum_{\gamma=1}^{s} b^{\rho\gamma} \cdot \delta q_i^{k,\gamma}$$

$$\overline{\delta v}_i^{k,\rho} = \overline{\delta v}_{\mathrm{par}(i)}^{k,\rho} + \dot{\overline{S}}_i^{k,\rho} \cdot \delta q_i^{k,\rho} + \overline{S}_i^{k,\rho} \cdot \delta \dot{q}_i^{k,\rho}$$

end for

end for

Algorithm B.2 Recursive Computation of the Newton Direction – Backward Pass

$\forall \alpha = 0, 1, \cdots, s, \forall \rho = 0, 1, \cdots, s$ and $\forall \nu = 0, 1, \cdots, s-1$,

$$D_i^{k,\alpha\rho} = \sigma^{\alpha\rho} \overline{M}_i^{k,\alpha} + \sum_{j \in \mathrm{chd}(i)} \Big(D_j^{k,\alpha\rho} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} X_j^{k,\gamma\rho} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} X_j^{k,\alpha\rho} \Big), \quad \text{(B.1a)}$$

$$G_i^{k,\alpha\nu} = \sum_{j \in \mathrm{chd}(i)} \Big(G_j^{k,\alpha\nu} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} Y_j^{k,\gamma\nu} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} Y_j^{k,\alpha\nu} \Big), \quad \text{(B.1b)}$$

$$l_i^{k,\alpha} = \sum_{j \in \mathrm{chd}(i)} \Big(l_j^{k,\alpha} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} y_j^{k,\gamma} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} y_j^{k,\alpha} \Big), \quad \text{(B.1c)}$$

$$\overline{\mu}_i^{k,\alpha} = \overline{M}_i^{k,\alpha} \overline{v}_i^{k,\alpha} + \sum_{j \in \mathrm{chd}(i)} \mu_j^{k,\alpha}$$

in which

$$\sigma^{\alpha\rho} = \begin{cases} 1 & \alpha = \rho, \\ 0 & \alpha \neq \rho \end{cases} \quad \text{and} \quad \overline{\sigma}^{\alpha 0} = \begin{cases} 1 & \alpha \neq 0, \\ 0 & \alpha = 0 \end{cases} \quad \text{(B.2)}$$

$\forall \alpha = 0, 1, \cdots, s-1, \forall \rho = 0, 1, \cdots, s$ and $\forall \nu = 0, 1, \cdots, s-1$,

$$\Pi_i^{k,\alpha\rho} = \sigma^{\alpha\rho} \mathbb{D}_2 \overline{F}_i^{k,\alpha} + \sum_{j \in \mathrm{chd}(i)} \Big(\Pi_j^{k,\alpha\rho} + \sum_{\gamma=1}^{s} \Phi_j^{k,\alpha\gamma} X_j^{k,\gamma\rho} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} X_j^{k,\alpha\rho} \Big), \quad \text{(B.3a)}$$

$$\Psi_i^{k,\alpha\nu} = \sigma^{\alpha\nu}\Big(\mathbb{D}_1\overline{F}_i^{k,\alpha} + \mathrm{ad}^D_{\overline{F}_i^{k,\alpha}} - \mathbb{D}_2\overline{F}_i^{k,\alpha}\mathrm{ad}_{\overline{v}_i^{k,\alpha}}\Big) + \sum_{j\in\mathrm{chd}(i)}\Big(\Psi_j^{k,\alpha\nu} + \sum_{\gamma=1}^{s}\Phi_j^{k,\alpha\gamma}Y_j^{k,\gamma\nu} - \overline{\sigma}^{\alpha 0}\mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}Y_j^{k,\alpha\nu}\Big), \quad \text{(B.3b)}$$

$$\zeta_i^{k,\alpha} = \sum_{j\in\mathrm{chd}(i)}\Big(\zeta_j^{k,\alpha} + \sum_{\gamma=1}^{s}\Phi_j^{k,\alpha\gamma}y_j^{k,\gamma} - \overline{\sigma}^{\alpha 0}\mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}y_j^{k,\alpha}\Big), \quad \text{(B.3c)}$$

$$\overline{\Gamma}_i^{k,\alpha} = \overline{F}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\overline{\Gamma}_j^{k,\alpha}$$

3: $\forall\alpha = 0, 1, \cdots, s$ and $\forall\gamma = 1, 2, \cdots, s$,

$$H_i^{k,\alpha\gamma} = D_i^{k,\alpha\gamma}\dot{\overline{S}}_i^{k,\gamma} + G_i^{k,\alpha\gamma}\overline{S}_i^{k,\gamma} + \frac{1}{\Delta t}\sum_{\rho=0}^{s} b^{\rho\gamma}D_i^{k,\alpha\rho}\overline{S}_i^{k,\rho}.$$

4: $\forall\alpha = 0, 1, \cdots, s-1$ and $\forall\gamma = 1, 2, \cdots, s$,

$$\Phi_i^{k,\alpha\gamma} = \Pi_i^{k,\alpha\gamma}\dot{\overline{S}}_i^{k,\gamma} + \Psi_i^{k,\alpha\gamma}\overline{S}_i^{k,\gamma} + \frac{1}{\Delta t}\sum_{\rho=0}^{s} b^{\rho\gamma}\Pi_i^{k,\alpha\rho}\overline{S}_i^{k,\rho}.$$

5: $\forall\alpha = 0, 1, \cdots, s-1, \forall\rho = 0, 1, \cdots, s$ and $\forall\nu = 0, 1, \cdots, s-1$,

$$\Theta_i^{k,\alpha\rho} = w^\alpha\Delta t\cdot\big({\dot{\overline{S}}_i^{k,\alpha}}^T D_i^{k,\alpha\rho} + \sigma^{\alpha\rho}{\overline{S}_i^{k,\alpha}}^T\mathrm{ad}^D_{\mu_i^{k,\alpha}}\big) + {\overline{S}_i^{k,\alpha}}^T\Pi_i^{k,\alpha\rho},$$

$$\Xi_i^{k,\alpha\nu} = w^\alpha\Delta t\cdot{\dot{\overline{S}}_i^{k,\alpha}}^T G_i^{k,\alpha\nu} + {\overline{S}_i^{k,\alpha}}^T\Psi_i^{k,\alpha\nu}.$$

6: $\forall\alpha = 0, 1, \cdots, s-1, \forall\rho = 0, 1, \cdots, s$ and $\forall\nu = 0, 1, \cdots, s-1$,

$$\overline{\Theta}_i^{k,\alpha\rho} = \Theta_i^{k,\alpha\rho} + \sum_{\beta=0}^{s} a^{\alpha\beta}{\overline{S}_i^{k,\beta}}^T D_i^{k,\beta\rho},$$

$$\overline{\Xi}_i^{k,\alpha\nu} = \Xi_i^{k,\alpha\nu} + \sum_{\beta=0}^{s} a^{\alpha\beta}{\overline{S}_i^{k,\beta}}^T G_i^{k,\beta\nu},$$

$$\overline{\xi}_i^{k,\alpha} = w^\alpha\Delta t\cdot{\dot{\overline{S}}_i^{k,\alpha}}^T l_i^{k,\alpha} + {\overline{S}_i^{k,\alpha}}^T\zeta_i^{k,\alpha} + \sum_{\beta=0}^{s} a^{\alpha\beta}{\overline{S}_i^{k,\beta}}^T l_i^{k,\beta}.$$

7: $\forall\alpha = 0, 1, \cdots, s-1$ and $\forall\gamma = 1, 2, \cdots, s$,

$$\Lambda_i^{k,\alpha\gamma} = w^\alpha\Delta t\cdot{\dot{\overline{S}}_i^{k,\alpha}}^T H_i^{k,\alpha\gamma} + {\overline{S}_i^{k,\alpha}}^T\Phi_i^{k,\alpha\gamma} + \sum_{\beta=0}^{s} a^{\alpha\beta}{\overline{S}_i^{k,\beta}}^T H_i^{k,\beta\gamma} + \sigma^{\alpha\gamma}\Big(\mathbb{D}_1 Q_i^{k,\alpha} + w^\alpha\Delta t\cdot{\overline{S}_i^{k,\alpha}}^T\mathrm{ad}^D_{\mu_i^{k,\alpha}}\dot{\overline{S}}_i^{k,\alpha}\Big) + \frac{1}{\Delta t}b^{\alpha\gamma}\cdot\mathbb{D}_2 Q_i^{k,\alpha}$$

with which $\Lambda_i^k = \big[\Lambda_i^{k,\alpha\gamma}\big] \in \mathbb{R}^{s\times s}$

8: $\forall\gamma = 1, 2, \cdots, s$ and $\forall\varrho = 0, 1, \cdots, s-1$, compute $\overline{\Lambda}_i^{k,\gamma\varrho}$ such that $\Lambda_i^{k^{-1}} = \left[\overline{\Lambda}_i^{k,\gamma\varrho}\right] \in \mathbb{R}^{s\times s}$

9: $\forall\gamma = 1, 2, \cdots, s, \forall\rho = 0, 1, \cdots, s$ and $\forall\nu = 1, 2, \cdots, s$

$$X_i^{k,\gamma\rho} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_i^{k,\gamma\varrho} \cdot \overline{\Theta}_i^{k,\varrho\rho},$$

$$Y_i^{k,\gamma\nu} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_i^{k,\gamma\varrho} \cdot \overline{\Xi}_i^{k,\varrho\nu},$$

$$y_i^{k,\gamma} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_i^{k,\gamma\varrho} \left(r_i^{k,\varrho} + \overline{\xi}_i^{k,\varrho}\right)$$

C Preliminaries

In this section, we present additional preliminaries used in Algorithms B.1 and B.2 and the proofs of Propositions 1 to 4. In Section C.1, we extend the contents of Section 2.3 for the computation of variations and derivatives. In Sections C.2 and C.3, we respectively introduce the notion of the spatial variation for spatial quantities and the differentiation on Lie groups, which are mainly used in Algorithms B.1 and B.2 and the proof of Proposition 2.

C.1 The Tree Representation Revisited

In addition to the computation of rigid body dynamics as those in Section 2.3, the tree representation can also be used to compute the variations and derivatives.

As is known, in the tree representation, the configuration $g_i \in SE(3)$ of rigid body i is

$$g_i = g_{\mathrm{par}(i)} g_{\mathrm{par}(i),i}(q_i) \tag{C.1}$$

in which $g_{\mathrm{par}(i),i}(q_i) = g_{\mathrm{par}(i),i}(0)\exp(\hat{S}_i q_i)$ and S_i is the body Jacobian of joint i with respect to frame $\{i\}$. In addition, the spatial Jacobian of joint i with respect to frame $\{0\}$ is

$$\overline{S}_i = \mathrm{Ad}_{g_i} S_i \tag{C.2}$$

in which S_i is constant by definition. Using Eqs. (C.1) and (C.2) as well as $\mathrm{Ad}_{g_i} S_i = \left(g_i \hat{S}_i g_i^{-1}\right)^\vee$, we obtain $\overline{\eta}_i = (\delta g_i g_i^{-1})^\vee$ as

$$\overline{\eta}_i = \overline{\eta}_{\mathrm{par}(i)} + \overline{S}_i \cdot \delta q_i, \tag{C.3}$$

or equivalently,

$$\overline{\eta}_i = \overline{S}_i \cdot \delta q_i + \sum_{j\in\mathrm{anc}(i)}^{n} \overline{S}_j \cdot \delta q_j \tag{C.4}$$

and furthermore,

$$\left(\frac{\partial g_i}{\partial q_j} g_i^{-1}\right)^\vee = \begin{cases} \overline{S}_j & j \in \text{anc}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{C.5a}$$

$$\left(\frac{\partial g_j}{\partial q_i} g_i^{-1}\right)^\vee = \begin{cases} \overline{S}_i & j \in \text{des}(i) \cup \{i\}, \\ 0 & \text{otherwise}. \end{cases} \tag{C.5b}$$

In addition, from Eqs. (C.2) and (C.3), $\delta \text{Ad}_{g_i} = \text{ad}_{\overline{\eta}_i} \text{Ad}_{g_i}$ and $\text{ad}_{\overline{S}_i} \overline{S}_i = 0$, we obtain

$$\delta \overline{S}_i = \text{ad}_{\overline{\eta}_i} \overline{S}_i = -\text{ad}_{\overline{S}_i} \overline{\eta}_i = \text{ad}_{\overline{\eta}_{\text{par}(i)}} \overline{S}_i = -\text{ad}_{\overline{S}_i} \overline{\eta}_{\text{par}(i)}. \tag{C.6}$$

Moreover, as a result of Eqs. (C.4) to (C.6), we further obtain

$$\frac{\partial \overline{S}_i}{\partial q_j} = \begin{cases} \text{ad}_{\overline{S}_j} \overline{S}_i & j \in \text{anc}(i), \\ 0 & \text{otherwise}, \end{cases} \tag{C.7a}$$

$$\frac{\partial \overline{S}_j}{\partial q_i} = \begin{cases} \text{ad}_{\overline{S}_i} \overline{S}_j & j \in \text{des}(i), \\ 0 & \text{otherwise}. \end{cases} \tag{C.7b}$$

Since the spatial velocity $\overline{v}_i$ of rigid body i is

$$\begin{aligned} \overline{v}_i &= \overline{S}_i \cdot \dot{q}_i + \sum_{j \in \text{anc}(i)} \overline{S}_j \cdot \dot{q}_j \\ &= \overline{v}_{\text{par}(i)} + \overline{S}_i \cdot \dot{q}_i, \end{aligned} \tag{C.8}$$

we obtain

$$\begin{aligned} \delta \overline{v}_i &= \delta \overline{S}_i \cdot \dot{q}_i + \overline{S}_i \cdot \delta \dot{q}_i + \sum_{j \in \text{anc}(i)} \left(\delta \overline{S}_j \cdot \dot{q}_j + \overline{S}_j \cdot \delta \dot{q}_j\right) \\ &= \delta \overline{v}_{\text{par}(i)} + \delta \overline{S}_i \cdot \dot{q}_i + \overline{S}_i \cdot \delta \dot{q}_i. \end{aligned}$$

Substitute Eq. (C.6) into the equation above, the result is

$$\begin{aligned} \delta \overline{v}_i &= \text{ad}_{\overline{\eta}_i} \overline{S}_i \cdot \dot{q}_i + \overline{S}_i \cdot \delta \dot{q}_i + \sum_{j \in \text{anc}(i)} \left(\text{ad}_{\overline{\eta}_j} \overline{S}_j \cdot \dot{q}_j + \overline{S}_j \cdot \delta \dot{q}_j\right) \\ &= \delta \overline{v}_{\text{par}(i)} + \text{ad}_{\overline{\eta}_i} \overline{S}_i \cdot \dot{q}_i + \overline{S}_i \cdot \delta \dot{q}_i. \end{aligned} \tag{C.9}$$

From Eqs. (C.6) to (C.9), we obtain

$$\frac{\partial \overline{v}_i}{\partial \dot{q}_j} = \begin{cases} S_j & j \in \text{anc}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{C.10a}$$

$$\frac{\partial \overline{v}_j}{\partial \dot{q}_i} = \begin{cases} S_i & j \in \text{des}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{C.10b}$$

and

$$\frac{\partial \overline{v}_i}{\partial q_j} = \begin{cases} \text{ad}_{\overline{S}_j} (\overline{v}_i - \overline{v}_j) & j \in \text{anc}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{C.11a}$$

$$\frac{\partial \overline{v}_j}{\partial q_i} = \begin{cases} \mathrm{ad}_{\overline{S}_i}(\overline{v}_j - \overline{v}_i) & j \in \mathrm{des}(i) \cup \{i\}, \\ 0 & \text{otherwise.} \end{cases} \tag{C.11b}$$

In addition, from Eqs. (C.2) and (C.8), $\mathrm{Ad}_{\dot{g}_i} = \mathrm{ad}_{\overline{v}_i}\mathrm{Ad}_{g_i}$ and $\mathrm{ad}_{\overline{S}_i}\overline{S}_i = 0$, we obtain

$$\dot{\overline{S}}_i = \mathrm{ad}_{\overline{v}_i}\overline{S}_i = -\mathrm{ad}_{\overline{S}_i}\overline{v}_i = \mathrm{ad}_{\overline{v}_{\mathrm{par}(i)}}\overline{S}_i = -\mathrm{ad}_{\overline{S}_i}\overline{v}_{\mathrm{par}(i)}. \tag{C.12}$$

As for the spatial inertia matrix $\overline{M}_i = \mathrm{Ad}_{g_i}^{-T} M_i \mathrm{Ad}_{g_i}^{-1}$, algebraic manipulation shows that

$$\delta\overline{M}_i = -\mathrm{ad}_{\overline{\eta}_i}^T \cdot \overline{M}_i - \overline{M}_i \cdot \mathrm{ad}_{\overline{\eta}_i}, \tag{C.13}$$

and from Eqs. (C.3) to (C.5) and Eq. (C.13), we obtain

$$\frac{\partial \overline{M}_i}{\partial q_j} = \begin{cases} -\mathrm{ad}_{\overline{S}_j}^T \overline{M}_i - \overline{M}_i \mathrm{ad}_{\overline{S}_j} & j \in \mathrm{anc}(i) \cup \{i\}, \\ 0 & \text{otherwise,} \end{cases} \tag{C.14a}$$

$$\frac{\partial \overline{M}_j}{\partial q_i} = \begin{cases} -\mathrm{ad}_{\overline{S}_i}^T \overline{M}_j - \overline{M}_j \mathrm{ad}_{\overline{S}_i} & j \in \mathrm{des}(i) \cup \{i\}, \\ 0 & \text{otherwise.} \end{cases} \tag{C.14b}$$

In Sections D.1 to D.4, Eq. (C.3) to (C.14) will be used to prove Propositions 1 to 4.

C.2 The Spatial Variation

In this subsection, we introduce the *spatial variation* $\overline{\delta}\overline{(\cdot)}$ that is used in Algorithms B.1 and B.2 and the proof of Proposition 2. Note that the notion of the spatial variation $\overline{\delta}\overline{(\cdot)}$ only applies to the spatial quantities $\overline{(\cdot)}$ of $T_eSE(3)$ or $T_e^*SE(3)$ that are described in the spatial frame.

If $\overline{a}, a \in T_eSE(3)$ are related as $\overline{a} = \mathrm{Ad}_g a$ in which $g \in SE(3)$, we have

$$\delta\overline{a} = \mathrm{Ad}_g \delta a + \mathrm{ad}_{\overline{\eta}}\overline{a}$$

in which $\overline{\eta} = (\delta g g^{-1})^\vee$. For numerical simplicity, it is sometimes preferable to have the variations of $\overline{a}$ and a still related by Ad_g. Therefore, we define the spatial variation $\overline{\delta}\overline{a}$ to be

$$\overline{\delta}\overline{a} = \delta\overline{a} - \mathrm{ad}_{\overline{\eta}}\overline{a} \tag{C.15}$$

such that $\overline{\delta}\overline{a} = \mathrm{Ad}_g \delta a$ as long as $\overline{a} = \mathrm{Ad}_g a$. In a similar way, if $\overline{b}^*, b^* \in T_e^*SE(3)$ are related as $\overline{b}^* = \mathrm{Ad}_g^{-T} b^*$, we obtain

$$\delta\overline{b}^* = \mathrm{Ad}_g^{-T}\delta b^* - \mathrm{ad}_{\overline{\eta}}^T \overline{b}^*.$$

Similar to Eq. (C.15), the spatial variation $\overline{\delta}\overline{b}^*$ is defined to be

$$\overline{\delta}\overline{b}^* = \delta\overline{b}^* + \mathrm{ad}_{\overline{\eta}}^T \overline{b}^* \tag{C.16}$$

such that $\overline{\delta}\,\overline{b}^* = \mathrm{Ad}_g^{-T}\delta b^*$ as long as $\overline{b}^* = \mathrm{Ad}_g^{-T} b^*$. In addition, note that $\delta\big(b^{*T}a\big) = \delta b^{*T} a + b^{*T}\delta a = \overline{\delta}\,\overline{b}^{*T}\overline{a} + \overline{b}^{*T}\overline{\delta}\overline{a}$ and $\delta(\overline{b}^{*T}\overline{a}) = \delta(b^{*T}a)$, we have

$$\delta(\overline{b}^{*T}\overline{a}) = \overline{\delta}\,\overline{b}^{*T}\overline{a} + \overline{b}^{*T}\overline{\delta}\overline{a}. \tag{C.17}$$

In general, the spatial variations $\overline{\delta}\,\overline{(\cdot)}$ are the infinitesimal changes of spatial quantities in either the Lie algebra $T_e SE(3)$ or the dual Lie algebra $T_e^* SE(3)$ after canceling out the influences of the frame change.

In Section 3, we have a number of spatial quantities that are defined in $T_e SE(3)$ and $T_e^* SE(3)$, whose spatial variations $\overline{\delta}\,\overline{(\cdot)}$ can be computed in the tree representation.

Following Eqs. (C.2), (C.6) and (C.15), for $\overline{S}_i^{k,\alpha} = \mathrm{Ad}_{g_i^{k,\alpha}} S_i$, the spatial variation $\overline{\delta}\,\overline{S}_i^{k,\alpha}$ is

$$\overline{\delta}\,\overline{S}_i^{k,\alpha} = 0 \tag{C.18}$$

though $\delta\overline{S}_i^{k,\alpha} = \mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{S}_i^{k,\alpha}$ is usually not zero. In addition, according to Eqs. (C.9) and (C.15), we have

$$\overline{\delta}\overline{v}_i^{k,\alpha} = \delta\overline{v}_{\mathrm{par}(i)}^{k,\alpha} + \mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{S}_i^{k,\alpha}\cdot\dot{q}_i^{k,\alpha} + \overline{S}_i^{k,\alpha}\cdot\delta\dot{q}_i^{k,\alpha} - \mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{v}_i^{k,\alpha}$$

Substitute Eqs. (C.3) and (C.8) into the equation above to expand $\mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{v}_i^{k,\alpha}$ and apply Eqs. (C.6) and (C.12), it can be shown that

$$\overline{\delta}\overline{v}_i^{k,\alpha} = \overline{\delta}\overline{v}_{\mathrm{par}(i)}^{k,\alpha} + \dot{\overline{S}}_i^{k,\alpha}\cdot\delta q_i^{k,\alpha} + \overline{S}_i^{k,\alpha}\cdot\delta\dot{q}^{k,\alpha}. \tag{C.19}$$

In terms of $\overline{\mu}_i^{k,\alpha}$, $\overline{\Gamma}_i^{k,\alpha}$ and $\overline{\Omega}_i^{k,\alpha}$ in Eq. (7), which are spatial quantities in $T_e^* SE(3)$, we can still implement the tree representation to compute the spatial variation. According to Definition 1, we have

$$\delta\overline{\mu}_i^{k,\alpha} = \delta(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \sum_{j\in\mathrm{chd}(i)}\delta\overline{\mu}_j^{k,\alpha}.$$

From Eq. (C.16), the spatial variation $\overline{\delta}\overline{\mu}_i^{k,\alpha}$ is

$$\overline{\delta}\overline{\mu}_i^{k,\alpha} = \delta(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \sum_{j\in\mathrm{chd}(i)}\delta\overline{\mu}_j^{k,\alpha} + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}\overline{\mu}_i^{k,\alpha}.$$

Using $\overline{\mu}_i^{k,\alpha} = \overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\overline{\mu}_j^{k,\alpha}$ and $\overline{\eta}_i^{k,\alpha} = \overline{\eta}_j^{k,\alpha} - \overline{S}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}$, we have

$$\begin{aligned}\overline{\delta}\overline{\mu}_i^{k,\alpha} = \delta(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \\ \sum_{j\in\mathrm{chd}(i)}\left(\delta\overline{\mu}_j^{k,\alpha} + \mathrm{ad}^T_{\overline{\eta}_j^{k,\alpha}}\overline{\mu}_j^{k,\alpha} - \mathrm{ad}^T_{\overline{S}_j^{k,\alpha}}\overline{\mu}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right)\end{aligned} \tag{C.20}$$

As a result of Eqs. (C.13) and (C.15), $\delta(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha})$ is

$$\begin{aligned}\delta(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}(\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha}) &= \overline{M}_i^{k,\alpha}(\delta\overline{v}_i^{k,\alpha} - \mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{v}_i^{k,\alpha}) \\ &= \overline{M}_i^{k,\alpha}\overline{\delta}\overline{v}_i^{k,\alpha}.\end{aligned} \tag{C.21}$$

From Eqs. (C.16) and (C.21) and $\mathrm{ad}^T_{\overline{S}_j^{k,\alpha}}\overline{\mu}_j^{k,\alpha} = \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}$, Eq. (C.20) is simplified to

$$\begin{aligned}\overline{\delta}\overline{\mu}_i^{k,\alpha} &= \overline{M}_i^{k,\alpha}\overline{\delta}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\overline{\delta}\overline{\mu}_j^{k,\alpha} - \mathrm{ad}^T_{\overline{S}_j^{k,\alpha}}\overline{\mu}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right) \\ &= \overline{M}_i^{k,\alpha}\overline{\delta}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\overline{\delta}\overline{\mu}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right).\end{aligned} \tag{C.22}$$

In a similar way, for the spatial variation $\overline{\delta}\overline{\Gamma}_i^{k,\alpha}$, we obtain

$$\begin{aligned}\overline{\delta}\overline{\Gamma}_i^{k,\alpha} &= \overline{\delta}\overline{F}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\overline{\delta}\overline{\Gamma}_j^{k,\alpha} - \mathrm{ad}^T_{\overline{S}_j^{k,\alpha}}\overline{\Gamma}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right) \\ &= \overline{\delta}\overline{F}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\overline{\delta}\overline{\Gamma}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right).\end{aligned} \tag{C.23}$$

As for $\overline{\Omega}_i^{k,\alpha} = w^\alpha\Delta t\cdot\mathrm{ad}^T_{\overline{v}_i^{k,\alpha}}\cdot\overline{\mu}_i^{k,\alpha} + \overline{\Gamma}_i^{k,\alpha}$, from Eqs. (C.15) and (C.16), algebraic manipulation shows that

$$\begin{aligned}\overline{\delta}\overline{\Omega}_i^{k,\alpha} &= \delta\overline{\Omega}_i^{k,\alpha} + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}\overline{\Omega}_i^{k,\alpha} \\ &= w^\alpha\Delta t\cdot\left(\mathrm{ad}^T_{\overline{v}_i^{k,\alpha}}\cdot\overline{\delta}\overline{\mu}_i^{k,\alpha} + \mathrm{ad}^T_{\overline{\delta}\overline{v}_i^{k,\alpha}}\overline{\mu}_i^{k,\alpha}\right) + \overline{\delta}\overline{\Gamma}_i^{k,\alpha} \\ &= w^\alpha\Delta t\cdot\left(\mathrm{ad}^T_{\overline{v}_i^{k,\alpha}}\cdot\overline{\delta}\overline{\mu}_i^{k,\alpha} + \mathrm{ad}^D_{\overline{\mu}_i^{k,\alpha}}\overline{\delta}\overline{v}_i^{k,\alpha}\right) + \overline{\delta}\overline{\Gamma}_i^{k,\alpha}.\end{aligned} \tag{C.24}$$

In Section D.2, Eqs. (C.18), (C.19) and (C.22) to (C.24) will be used to prove Proposition 2.

C.3 Differentiation on Lie Groups

For an analytical function $f:\mathbb{R}^n\to\mathbb{R}$, the directional derivative at $x\in\mathbb{R}^n$ in the direction δx is defined to be

$$\mathbb{D}f(x)\cdot\delta x = \left.\frac{\mathrm{d}}{\mathrm{d}t}f(x+t\cdot\delta x)\right|_{t=0}$$

in which $\mathbb{D}f(x) = \begin{bmatrix}\frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n}\end{bmatrix}^T\in\mathbb{R}^n$.

In a similar way, we might define the directional derivative on Lie groups using the Lie algebra and the exponential map as follows.

Definition C.1. *If G is a n-dimensional smooth Lie group and $f: G \longrightarrow \mathbb{R}$ is a smooth function on G, the directional derivative at $g \in G$ in the direction $\overline{\eta} = \delta g g^{-1} \in T_eG$ is defined to be*

$$\mathbb{D}f(g) \cdot \overline{\eta} = \frac{\mathrm{d}}{\mathrm{d}t} f\left(\exp\left(t \cdot \overline{\eta}\right) g\right)\bigg|_{t=0}.$$

Moreover, if $\overline{e}_1,\ \overline{e}_2,\ \cdots,\ \overline{e}_n$ is a basis for the Lie algebra T_eG, then $\mathbb{D}f(g)$ can be explicitly written as

$$\mathbb{D}f(g) = \frac{\mathrm{d}}{\mathrm{d}t}\left[f\left(\exp\left(t \cdot \overline{e}_1\right) g\right) \ \ f\left(\exp\left(t \cdot \overline{e}_2\right) g\right) \ \ \cdots \ \ f\left(\exp\left(t \cdot \overline{e}_n\right) g\right)\right]^T\bigg|_{t=0}.$$

In regard to Lie group theory, $\mathbb{R}^n$ is also a smooth Lie group for which the binary operation is addition, the Lie algebra is itself and the exponential map is the identity map. Furthermore, the definition of directional derivatives on Lie groups in Definition C.1 is consistent with the definition of directional derivatives in $\mathbb{R}^n$. Therefore, it is without loss of any generality to interpret all the quantities in this paper as elements of Lie groups and all the derivatives in this paper as derivatives on Lie groups that are defined by Definition C.1.

In this paper, following the notation in multivariate calculus, if $f: G_1 \times G_2 \times \cdots \times G_d \rightarrow \mathbb{R}$ is a smooth function in which $G_1, G_2, \cdots, G_d$ are Lie groups, we use $\mathbb{D}_i f$ to denote the derivative with respect to G_i. In particular, for $\overline{F}_i^{k,\alpha} = \overline{F}_i^{k,\alpha}(g_i^{k,\alpha}, \overline{v}_i^{k,\alpha}, u_i^{k,\alpha})$ that is used for the computation of the Newton direction in Algorithm B.2, note that $\mathbb{D}_1\overline{F}_i^{k,\alpha}$ is the derivative with respect to $g_i^{k,\alpha}$ and $\mathbb{D}_2\overline{F}_i^{k,\alpha}$ is the derivative with respect to $\overline{v}_i^{k,\alpha}$.

D Proof of Propositions

In this section, we review and prove Propositions 1 to 4 in [1] though these proofs are not necessary for implementation.

D.1 Proof of Proposition 1

In Section 3.1, we define the discrete articulated body momentum and discrete articulated body impulse are respectively as follows.

Definition 1. *The discrete articulated body momentum $\overline{\mu}_i^{k,\alpha} \in \mathbb{R}^6$ for articulated body i is defined to be*

$$\overline{\mu}_i^{k,\alpha} = \overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha} + \sum_{j \in \mathrm{chd}(i)} \overline{\mu}_j^{k,\alpha} \qquad \forall \alpha = 0,\, 1, \cdots,\, s \tag{D.1}$$

in which $\overline{M}_i^{k,\alpha}$ and $\overline{v}_i^{k,\alpha}$ are respectively the spatial inertia matrix and spatial velocity of rigid body i.

Definition 2. *Suppose $\overline{F}_i(t) \in \mathbb{R}^6$ is the sum of all the wrenches directly acting on rigid body i, which does not include those applied or transmitted through the joints that are connected to rigid body i. The discrete articulated body impulse $\overline{\Gamma}_i^{k,\alpha} \in \mathbb{R}^6$ for articulated body i is defined to be*

$$\overline{\Gamma}_i^{k,\alpha} = \overline{F}_i^{k,\alpha} + \sum_{j\in \mathrm{chd}(i)} \overline{\Gamma}_j^{k,\alpha} \tag{D.2}$$

in which $\overline{F}_i^{k,\alpha} = \omega^\alpha \overline{F}_i(t^{k,\alpha})\Delta t \in \mathbb{R}^6$ is the discrete impulse acting on rigid body i. Note that $\overline{F}_i(t)$, $\overline{F}_i^{k,\alpha}$ and $\overline{\Gamma}_i^{k,\alpha}$ are expressed in frame $\{0\}$.

The DEL equations Eq. (5) can be recursively evaluated with $\overline{\mu}_i^{k,\alpha}$ and $\overline{F}_i^{k,\alpha}$ as Proposition 1 indicates.

Proposition 1. *If $Q_i(t) \in \mathbb{R}$ is the sum of all joint forces applied to joint i and $p^k = \left[p_1^k\ p_2^k\ \cdots\ p_n^k\right]^T \in \mathbb{R}^n$ is the discrete momentum, the DEL equations Eq.* (5) *can be evaluated as*

$$r_i^{k,0} = p_i^k + \overline{S}_i^{k,0^T} \cdot \overline{\Omega}_i^{k,0} + \sum_{\beta=0}^{s} a^{0\beta} \overline{S}_i^{k,\beta^T} \cdot \overline{\mu}_i^{k,\beta} + Q_i^{k,0}, \tag{D.3a}$$

$$r_i^{k,\alpha} = \overline{S}_i^{k,\alpha^T} \cdot \overline{\Omega}_i^{k,\alpha} + \sum_{\beta=0}^{s} a^{\alpha\beta} \overline{S}_i^{k,\beta^T} \cdot \overline{\mu}_i^{k,\beta} + Q_i^{k,\alpha} \quad \forall \alpha = 1, \cdots, s-1, \tag{D.3b}$$

$$p_i^{k+1} = \overline{S}_i^{k,s^T} \cdot \overline{\Omega}_i^{k,s} + \sum_{\beta=0}^{s} a^{s\beta} \overline{S}_i^{k,\beta^T} \cdot \overline{\mu}_i^{k,\beta} + Q_i^{k,s} \tag{D.3c}$$

in which $r_i^{k,\alpha}$ is the residue of the DEL equations Eqs. (5a) *and* (5b)*, $a^{\alpha\beta} = w^\beta b^{\beta\alpha}$, $\overline{\Omega}_i^{k,\alpha} = w^\alpha \Delta t \cdot \mathrm{ad}^T_{\overline{v}_i^{k,\alpha}} \cdot \overline{\mu}_i^{k,\alpha} + \overline{\Gamma}_i^{k,\alpha}$, and $Q_i^{k,\alpha} = \omega^\alpha Q_i(t^{k,\alpha})\Delta t$ is the discrete joint force applied to joint i.*

Proof. The Lagrangian of a mechanical system is defined to be

$$\mathcal{L}(q, \dot{q}) = K(q, \dot{q}) - V(q) \tag{D.4}$$

in which $K(q, \dot{q})$ is the kinetic energy and $V(q)$ is the potential energy. It is by the definition of $\overline{F}_i(t)$ and $Q_i(t)$ that

$$\int_0^T \mathcal{F}(t) \cdot \delta q dt - \delta \int_0^T V(q) dt = \int_0^T \sum_{i=1}^{n} \overline{F}_i(t) \cdot \overline{\eta}_i dt + \int_0^T \sum_{i=1}^{n} Q_i(t) \cdot \delta q_i dt$$

in which $\overline{\eta}_i = (\delta g_i g_i^{-1})^\vee$. Therefore, the Lagrange-d'Alembert principle Eq. (1) is equivalent to

$$\delta \mathfrak{S} = \delta \int_0^T K(q, \dot{q}) dt + \int_0^T \sum_{i=1}^{n} \overline{F}_i(t) \cdot \overline{\eta}_i dt + \int_0^T \sum_{i=1}^{n} Q_i(t) \cdot \delta q_i dt = 0. \tag{D.5}$$

As a result of Eqs. (3) and (D.5), we have

$$\sum_{k=0}^{N-1}\sum_{\alpha=0}^{s} w^\alpha \sum_{i=1}^{n}\Big[\Big\langle \tfrac{\partial K}{\partial q_i}(q^{k,\alpha},\dot q^{k,\alpha}),\delta q_i^{k,\alpha}\Big\rangle + \Big\langle \tfrac{\partial K}{\partial \dot q_i}(q^{k,\alpha},\dot q^{k,\alpha}),\delta \dot q_i^{k,\alpha}\Big\rangle + \langle \overline{F}_i(t^{k,\alpha}),\overline{\eta}_i^{k,\alpha}\rangle + \langle Q_i(t^{k,\alpha}),\delta q_i^{k,\alpha}\rangle\Big]\Delta t = 0. \quad \text{(D.6)}$$

Note that the kinetic energy $K(q^{k,\alpha},\dot q^{k,\alpha})$ is

$$K(q^{k,\alpha},\dot q^{k,\alpha}) = \frac{1}{2}\sum_{j=1}^{n}\overline{v}_j^{k,\alpha\,T}\overline{M}_j^{k,\alpha}\overline{v}_j^{k,\alpha} \quad \text{(D.7)}$$

in which $\overline{M}_i^{k,\alpha}\in\mathbb{R}^{6\times 6}$ is the spatial inertia matrix and $\overline{v}_i^{k,\alpha}\in\mathbb{R}^6$ is the spatial velocity. Using Eqs. (C.10b), (D.1) and (D.7), we obtain

$$\begin{aligned}\frac{\partial K}{\partial \dot q_i}(q^{k,\alpha},\dot q^{k,\alpha}) =& \sum_{j=1}^{n}\frac{\partial \overline{v}_j^{k,\alpha}}{\partial \dot q_i}^{T}\overline{M}_j^{k,\alpha}\overline{v}_j^{k,\alpha}\\ =&\overline{S}_i^{k,\alpha\,T}\overline{M}_i^{k,\alpha}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{des}(i)}\overline{S}_i^{k,\alpha\,T}\overline{M}_j^{k,\alpha}\overline{v}_j^{k,\alpha}\\ =&\overline{S}_i^{k,\alpha\,T}\overline{\mu}_i^{k,\alpha}.\end{aligned} \quad \text{(D.8)}$$

In a similar way, as a result of Eqs. (C.14b), (C.11b), (C.12), (D.1) and (D.7), a tedious but straightforward algebraic manipulation results in

$$\begin{aligned}\frac{\partial K}{\partial q_i}(q^{k,\alpha},\dot q^{k,\alpha}) =& \sum_{j\in\mathrm{des}(i)\cup\{i\}}\Big[\mathrm{ad}_{\overline{S}_i^{k,\alpha}}(\overline{v}_j^{k,\alpha}-\overline{v}_i^{k,\alpha}) - \mathrm{ad}_{\overline{S}_i^{k,\alpha}}\overline{v}_j^{k,\alpha}\Big]^T\overline{M}_j^{k,\alpha}v_j^{k,\alpha}\\ =&S_i^{k,\alpha\,T}\mathrm{ad}_{\overline{v}_i}^{T}\cdot\overline{\mu}_i^{k,\alpha}\\ =&\dot{\overline{S}}_i^{k,\alpha\,T}\overline{\mu}_i^{k,\alpha}.\end{aligned} \quad \text{(D.9)}$$

In addition, using Eqs. (C.4) and (D.2) and $\overline{F}_i^{k,\alpha} = w^\alpha\overline{F}_i(t^{k,\alpha})\Delta t$, we obtain

$$\begin{aligned}\sum_{i=1}^{n}\langle w^\alpha\overline{F}_i(t^{k,\alpha})\Delta t,\overline{\eta}_i^{k,\alpha}\rangle =& \sum_{i=1}^{n}\langle w^\alpha\overline{F}_i(t^{k,\alpha})\Delta t,\overline{S}_i^{k,\alpha}\cdot\delta q_i^{k,\alpha} + \sum_{j\in\mathrm{anc}(i)}\overline{S}_j^{k,\alpha}\cdot q_j^{k,\alpha}\rangle\\ =&\sum_{i=1}^{n}\langle\overline{F}_i^{k,\alpha} + \sum_{j\in\mathrm{des}(i)}\overline{F}_j^{k,\alpha},\overline{S}_i^{k,\alpha}\cdot\delta q_i^{k,\alpha}\rangle\\ =&\sum_{i=1}^{n}\langle\overline{\Gamma}_i^{k,\alpha},\overline{S}_i^{k,\alpha}\cdot\delta q_i^{k,\alpha}\rangle\\ =&\sum_{i=1}^{n}\langle\overline{S}_i^{k,\alpha\,T}\overline{\Gamma}_i^{k,\alpha},\delta q_j^{k,\alpha}\rangle.\end{aligned} \quad \text{(D.10)}$$

From Eq. (2), we obtain

$$\delta\dot{q}_i^{k,\alpha} = \frac{1}{\Delta t}\sum_{\beta=0}^{s} b^{\alpha\beta}\cdot\delta q_i^{k,\beta}. \tag{D.11}$$

Substituting Eqs. (D.8) to (D.10) into Eq. (D.6) and simplifying the resulting equation with Eq. (D.11) as well as the chain rule, we obtain

$$\sum_{k=0}^{N-1}\sum_{\alpha=0}^{s}\sum_{i=1}^{n}\langle \overline{S}_i^{k,\alpha\,T}\cdot\overline{\Omega}_i^{k,\alpha} + \sum_{\beta=0}^{s} a^{\alpha\beta}\overline{S}_i^{k,\beta\,T}\cdot\overline{\mu}_i^{k,\beta} + Q_i^{k,\alpha}, \delta q_i^{k,\alpha}\rangle = 0$$

in which $a^{\alpha\beta} = w^{\beta} b^{\beta\alpha}$, $\overline{\Omega}_i^{k,\alpha} = w^{\alpha}\Delta t\cdot\mathrm{ad}^T_{\overline{v}_i^{k,\alpha}}\cdot\overline{\mu}_i^{k,\alpha} + \overline{\Gamma}_i^{k,\alpha}$ and $Q_i^{k,\alpha} = \omega^{\alpha} Q_i(t^{k,\alpha})\Delta t$. The equation above is equivalent to requiring

$$p_i^k + \overline{S}_i^{k,0\,T}\cdot\overline{\Omega}_i^{k,0} + \sum_{\beta=0}^{s} a^{0\beta}\overline{S}_i^{k,\beta\,T}\cdot\overline{\mu}_i^{k,\beta} + Q_i^{k,0} = 0,$$

$$\overline{S}_i^{k,\alpha\,T}\cdot\overline{\Omega}_i^{k,\alpha} + \sum_{\beta=0}^{s} a^{\alpha\beta}\overline{S}_i^{k,\beta\,T}\cdot\overline{\mu}_i^{k,\beta} + Q_i^{k,\alpha} = 0 \quad \forall\alpha = 1,\cdots,s-1,$$

$$p_i^{k+1} = \overline{S}_i^{k,s\,T}\cdot\overline{\Omega}_i^{k,s} + \sum_{\beta=0}^{s} a^{s\beta}\overline{S}_i^{k,\beta\,T}\cdot\overline{\mu}_i^{k,\beta} + Q_i^{k,s}.$$

This completes the proof. □

D.2 Proof of Proposition 2

In Section 3.2, we make the assumption on the discrete impulse $\overline{F}_i^{k,\alpha}$ and discrete joint force $Q_i^{k,\alpha}$ as follows.

Assumption 1. *Let $u(t)$ be control inputs of the mechanical system, we assume that the discrete impulse $\overline{F}_i^{k,\alpha}$ and discrete joint force $Q_i^{k,\alpha}$ can be respectively formulated as $\overline{F}_i^{k,\alpha} = \overline{F}_i^{k,\alpha}(g_i^{k,\alpha}, \overline{v}_i^{k,\alpha}, u^{k,\alpha})$ and $Q_i^{k,\alpha} = Q_i^{k,\alpha}(q_i^{k,\alpha}, \dot{q}_i^{k,\alpha}, u^{k,\alpha})$ in which $u^{k,\alpha} = u(t^{k,\alpha})$.*

From the notion of the spatial variation in Section C.2, we have the following proposition for the Newton direction computation, which is later used in the proof of Proposition 2.

Proposition D.1. *If $\delta q_i^{k,\alpha}$ is the Newton direction for $q_i^{k,\alpha}$, $r_i^{k,\alpha}$ is the residue of the DEL equations Eqs.* (7a) *and* (7b)*, and Assumption 1 holds, the computation of the Newton direction $\delta q_i^{k,\alpha}$ is equivalent to requiring*

$$\overline{\delta}\overline{\mu}_i^{k,\alpha} = \overline{M}_i^{k,\alpha}\overline{\delta}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\overline{\delta}\overline{\mu}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right)$$
$$\forall\alpha = 0,\,1,\,\cdots,\,s, \tag{D.12a}$$

$$\bar{\delta}\overline{\Gamma}_i^{k,\alpha} = \left(\mathbb{D}_1\overline{F}_i^{k,\alpha} + \mathrm{ad}^D_{\overline{F}_i^{k,\alpha}} - \mathrm{ad}_{\overline{v}_i^{k,\alpha}}\right)\cdot\overline{\eta}_i^{k,\alpha} + \mathbb{D}_2\overline{F}_i^{k,\alpha}\cdot\bar{\delta}\overline{v}_i^{k,\alpha} + \sum_{j\in\mathrm{chd}(i)}\left(\bar{\delta}\overline{\Gamma}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}\cdot\delta q_j^{k,\alpha}\right) \quad \forall\alpha = 0,\,1,\,\cdots,\,s-1, \tag{D.12b}$$

$$\bar{\delta}\overline{\Omega}_i^{k,\alpha} = \omega^\alpha \Delta t\cdot\left(\mathrm{ad}^T_{\overline{v}_i^{k,\alpha}}\cdot\bar{\delta}\overline{\mu}_i^{k,\alpha} + \mathrm{ad}^D_{\overline{\mu}_i^{k,\alpha}}\bar{\delta}\overline{v}_i^{k,\alpha}\right) + \bar{\delta}\overline{\Gamma}_i^{k,\alpha} \quad \forall\alpha = 0,\,1,\,\cdots,\,s-1, \tag{D.12c}$$

$$\overline{S}_i^{k,\alpha^T}\bar{\delta}\overline{\Omega}_i^{k,\alpha} + \sum_{\beta=0}^{s} a^{\alpha\beta}\overline{S}_i^{k,\beta^T}\bar{\delta}\overline{\mu}_i^{k,\beta} + \mathbb{D}_1 Q_i^{k,\alpha}\cdot\delta q_i^{k,\alpha} + \mathbb{D}_2 Q_i^{k,\alpha}\cdot\delta\dot{q}_i^{k,\alpha} = -r_i^{k,\alpha} \quad \forall\alpha = 0,\,1,\,\cdots,\,s-1. \tag{D.12d}$$

in which $\bar{\delta}\overline{v}_i^{k,\alpha}$, $\bar{\delta}\overline{\mu}_i^{k,\alpha}$, $\bar{\delta}\overline{\Gamma}_i^{k,\alpha}$ and $\bar{\delta}\overline{\Omega}_i^{k,\alpha}$ are the spatial variations of $\overline{v}_i^{k,\alpha}$, $\overline{\mu}_i^{k,\alpha}$, $\overline{\Gamma}_i^{k,\alpha}$ and $\overline{\Omega}_i^{k,\alpha}$, respectively. Note that $\delta q_i^{k,0} = 0$ and $\overline{\eta}_i^{k,0} = 0$ though $\bar{\delta}\overline{v}_i^{k,0} \neq 0$.

Proof. Eqs. (D.12a) and (D.12c) are respectively the same as Eqs. (C.22) and (C.24), thus we only need to prove Eqs. (D.12b) and (D.12d).

From Assumption 1, we have $\overline{F}_i^{k,\alpha} = \overline{F}_i^{k,\alpha}(g_i^{k,\alpha}, \overline{v}_i^{k,\alpha}, u^{k,\alpha})$, and since $\delta u_i^{k,\alpha} = 0$, we obtain $\delta\overline{F}_i^{k,\alpha}$ as

$$\delta\overline{F}_i^{k,\alpha} = \mathbb{D}_1\overline{F}_i^{k,\alpha}\cdot\overline{\eta}_i^{k,\alpha} + \mathbb{D}_2\overline{F}_i^{k,\alpha}\cdot\delta\overline{v}_i^{k,\alpha}.$$

According to Eq. (C.16), the spatial variation $\bar{\delta}\overline{F}_i^{k,\alpha}$ is

$$\bar{\delta}\overline{F}_i^{k,\alpha} = \mathbb{D}_1\overline{F}_i^{k,\alpha}\cdot\overline{\eta}_i^{k,\alpha} + \mathbb{D}_2\overline{F}_i^{k,\alpha}\cdot\delta\overline{v}_i^{k,\alpha} + \mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}\overline{F}_i^{k,\alpha}.$$

Since $\delta\overline{v}_i^{k,\alpha} = \bar{\delta}\overline{v}_i^{k,\alpha} + \mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{v}_i^{k,\alpha}$, $\mathrm{ad}_{\overline{v}_i^{k,\alpha}}\overline{\eta}_i^{k,\alpha} = -\mathrm{ad}_{\overline{\eta}_i^{k,\alpha}}\overline{v}_i^{k,\alpha}$ as well as $\mathrm{ad}^T_{\overline{\eta}_i^{k,\alpha}}\overline{F}_i^{k,\alpha} = \mathrm{ad}^D_{\overline{F}_i^{k,\alpha}}\overline{\eta}_i^{k,\alpha}$, the equation above is equivalent to

$$\bar{\delta}\overline{F}_i^{k,\alpha} = \left(\mathbb{D}_1\overline{F}_i^{k,\alpha} + \mathrm{ad}^D_{\overline{F}_i^{k,\alpha}} - \mathbb{D}_2\overline{F}_i^{k,\alpha}\mathrm{ad}_{\overline{v}_i^{k,\alpha}}\right)\cdot\overline{\eta}_i^{k,\alpha} + \mathbb{D}_2\overline{F}_i^{k,\alpha}\cdot\bar{\delta}\overline{v}_i^{k,\alpha}.$$

Substitute the equation above into Eq. (C.23), the result of which is Eq. (D.12b).

As for the proof of Eq. (D.12d), from Eqs. (7a) and (7b), the Newton direction $\delta q_i^{k,\alpha}$ requires that

$$\delta\left(S_i^{k,\alpha^T}\overline{\Omega}_i\right) + \sum_{\beta=0}^{s} a^{\alpha\beta}\delta\left(S_i^{k,\beta^T}\overline{\mu}_i^{k,\beta}\right) + \mathbb{D}_1 Q_i^{k,\alpha}\cdot\delta q_i^{k,\alpha} + \mathbb{D}_2 Q_i^{k,\alpha}\cdot\delta\dot{q}_i^{k,\alpha} = -r_i^{k,\alpha} \quad \forall\alpha = 0,\,1,\,\cdots,\,s-1. \tag{D.13}$$

As a result of Eqs. (C.17) and (C.18), we have $\delta\left(\overline{S}_i^{k,\alpha^T}\overline{\mu}_i^{k,\alpha}\right) = \overline{S}_i^{k,\alpha^T}\bar{\delta}\overline{\mu}_i^{k,\alpha}$ and $\delta\left(\overline{S}_i^{k,\alpha^T}\overline{\Omega}_i^{k,\alpha}\right) = \overline{S}_i^{k,\alpha^T}\bar{\delta}\overline{\Omega}_i^{k,\alpha}$, with which and Eq. (D.13), we obtain Eq. (D.12d). This completes the proof. □

In Section 3.2, Proposition 2 to compute the Newton direction is stated as follows, for which note that the higher-order variational integrator has $s+1$ control points and the mechanical system has n degrees of freedom.

Proposition 2. *For higher-order variational integrators of unconstrained mechanical systems, if Assumption 1 holds and $\mathcal{J}^{k^{-1}}(\overline{q}^k)$ exists, the Newton direction $\delta\overline{q}^k = -\mathcal{J}^{k^{-1}}(\overline{q}^k)\cdot r^k$ can be computed with Algorithm B.1 in $O(s^3 n)$ time.*

Proof. The proof consists of proving the correctness and the $O(n)$ complexity of the algorithms.

For each $j\in\operatorname{chd}(i)$, we suppose that there exists $D_j^{k,\alpha\rho}$, $G_j^{k,\alpha\nu}$, $l_j^{k,\alpha}$ and $\Pi_j^{k,\alpha\rho}$, $\Psi_j^{k,\alpha\nu}$, $\zeta_j^{k,\alpha}$ such that

$$\overline{\delta}\overline{\mu}_j^{k,\alpha} = \sum_{\rho=0}^{s} D_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_j^{k,\rho} + \sum_{\nu=1}^{s} G_j^{k,\alpha\nu}\cdot\overline{\eta}_j^{k,\nu} + l_j^{k,\alpha} \quad \forall\alpha = 0,\,1,\,\cdots,\,s, \tag{D.14}$$

$$\overline{\delta}\overline{\Gamma}_j^{k,\alpha} = \sum_{\rho=0}^{s} \Pi_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_j^{k,\rho} + \sum_{\nu=1}^{s} \Psi_j^{k,\alpha\nu}\cdot\overline{\eta}_j^{k,\nu} + \zeta_j^{k,\alpha} \quad \forall\alpha = 0,\,1,\,\cdots,\,s-1. \tag{D.15}$$

According to Eqs. (C.3), (C.19) and (D.11), $\overline{\delta}\overline{v}_j^{k,\rho}$ and $\overline{\eta}_j^{k,\nu}$ can be respectively computed as

$$\overline{\eta}_j^{k,\nu} = \overline{\eta}_i^{k,\nu} + \overline{S}_j^{k,\nu}\cdot\delta q_j^{k,\nu} \tag{D.16}$$

and

$$\overline{\delta}\overline{v}_j^{k,\rho} = \overline{\delta}\overline{v}_i^{k,\rho} + \dot{\overline{S}}_j^{k,\rho}\cdot\delta q_j^{k,\rho} + \frac{1}{\Delta t}\overline{S}_j^{k,\rho}\sum_{\gamma=1}^{s} b^{\rho\gamma}\cdot\delta q_j^{k,\gamma} \tag{D.17}$$

for which note that $\delta q_j^{k,0}=0$. Substitute Eqs. (D.16) and (D.17) into Eq. (D.14), algebraic manipulation shows that

$$\overline{\delta}\overline{\mu}_j^{k,\alpha} = \sum_{\rho=0}^{s} D_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} G_j^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu} + l_j^{k,\alpha} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma}\delta q_j^{k,\gamma}, \tag{D.18}$$

in which

$$H_j^{k,\alpha\gamma} = D_j^{k,\alpha\gamma}\dot{\overline{S}}_j^{k,\gamma} + G_j^{k,\alpha\gamma}\overline{S}_j^{k,\gamma} + \frac{1}{\Delta t}\sum_{\rho=0}^{s} b^{\rho\gamma} D_j^{k,\alpha\rho}\overline{S}_j^{k,\rho}.$$

In a similar way, using Eqs. (D.15) to (D.17), we also have

$$\overline{\delta}\overline{\Gamma}_j^{k,\alpha} = \sum_{\rho=0}^{s} \Pi_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} \Psi_j^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu} + \zeta^{k,\alpha} + \sum_{\gamma=1}^{s} \Phi_j^{k,\alpha\gamma}\delta q_j^{k,\gamma} \tag{D.19}$$

in which

$$\varPhi_j^{k,\alpha\gamma}=\varPi_j^{k,\alpha\gamma}\dot{\overline{S}}_j^{k,\gamma}+\varPsi_j^{k,\alpha\gamma}\overline{S}_j^{k,\gamma}+\frac{1}{\varDelta t}\sum_{\rho=0}^{s}b^{\rho\gamma}\varPi_j^{k,\alpha\rho}\overline{S}_j^{k,\rho}.$$

From Eqs. (C.12), (C.24) and (D.17) to (D.19) and

$$\overline{S}_j^{k,\alpha^T}\mathrm{ad}^T_{\overline{S}_j^{k,\alpha}}\overline{\mu}_j^{k,\alpha}=\overline{S}_j^{k,\alpha^T}\mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\overline{S}_j^{k,\alpha}=0,$$

we obtain

$$\overline{S}_j^{k,\alpha^T}\overline{\delta}\,\overline{\varOmega}_j^{k,\alpha}=\sum_{\rho=0}^{s}\varTheta_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho}+\sum_{\nu=1}^{s}\varXi^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu}+\xi_j^{k,\alpha}\tag{D.20}$$

in which

$$\begin{aligned}\varTheta_j^{k,\alpha\rho}&=w^\alpha\varDelta t\cdot\big(\dot{\overline{S}}_j^{k,\alpha^T}D_j^{k,\alpha\rho}+\sigma^{\alpha\rho}\overline{S}_j^{k,\alpha^T}\mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\big)+\overline{S}_j^{k,\alpha^T}\varPi_j^{k,\alpha\rho},\\ \varXi_j^{k,\alpha\nu}&=w^\alpha\varDelta t\cdot\dot{\overline{S}}_j^{k,\alpha^T}G_j^{k,\alpha\nu}+\overline{S}_j^{k,\alpha^T}\varPsi_j^{k,\alpha\nu},\\ \xi_j^{k,\alpha}&=w^\alpha\varDelta t\cdot\dot{\overline{S}}_j^{k,\alpha^T}l_j^{k,\alpha}+\overline{S}_j^{k,\alpha^T}\zeta_j^{k,\alpha}+\sum_{\gamma=1}^{s}\Big[w^\alpha\varDelta t\cdot\big(\dot{\overline{S}}_j{}^{k,\alpha^T}H_j^{k,\alpha\gamma}+\\ &\qquad\sigma^{\alpha\gamma}\overline{S}_j^{k,\alpha^T}\mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\dot{\overline{S}}_j^{k,\alpha}\big)+\overline{S}_j^{k,\alpha^T}\varPhi_j^{k,\alpha\gamma}\Big]\delta q_j^{k,\gamma},\end{aligned}$$

and note that $\sigma^{\alpha\rho}$ is given in Eq. (B.2) of Algorithm B.2. Substituting Eqs. (D.11), (D.18) and (D.20) into Eq. (D.12d), we obtain

$$\sum_{\rho=0}^{s}\overline{\varTheta}_j^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho}+\sum_{\nu=1}^{s}\overline{\varXi}_j^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu}+\overline{\xi}_j^{k,\alpha}+\sum_{\gamma=1}^{s}\varLambda_j^{k,\alpha\gamma}\cdot\delta q_j^{k,\gamma}=-r_j^{k,\alpha}$$

$$\forall\alpha=0,\,1,\,\cdots,\,s-1.\tag{D.21}$$

in which

$$\begin{aligned}\overline{\varTheta}_j^{k,\alpha\rho}&=\varTheta_j^{k,\alpha\rho}+\sum_{\beta=0}^{s}a^{\alpha\beta}\overline{S}_j^{k,\beta^T}D_j^{k,\beta\rho},\\ \overline{\varXi}_j^{k,\alpha\nu}&=\varXi_j^{k,\alpha\nu}+\sum_{\beta=0}^{s}a^{\alpha\beta}\overline{S}_j^{k,\beta^T}G_j^{k,\beta\nu},\\ \overline{\xi}_j^{k,\alpha}&=w^\alpha\varDelta t\cdot\dot{\overline{S}}_j^{k,\alpha^T}l_j^{k,\alpha}+\overline{S}_j^{k,\alpha^T}\zeta_j^{k,\alpha}+\sum_{\beta=0}^{s}a^{\alpha\beta}\overline{S}_j^{k,\beta^T}l_j^{k,\beta},\\ \varLambda_j^{k,\alpha\gamma}&=w^\alpha\varDelta t\cdot\dot{\overline{S}}_j^{k,\alpha^T}H_j^{k,\alpha\gamma}+\overline{S}_j^{k,\alpha^T}\varPhi_j^{k,\alpha\gamma}+\sum_{\beta=0}^{s}a^{\alpha\beta}\overline{S}_j^{k,\beta^T}H_j^{k,\beta\gamma}+\\ &\qquad\sigma^{\alpha\gamma}\left(\mathbb{D}_1Q_j^{k,\alpha}+w^\alpha\varDelta t\cdot\overline{S}_j^{k,\alpha^T}\mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}}\dot{\overline{S}}_j^{k,\alpha}\right)+\frac{1}{\varDelta t}b^{\alpha\gamma}\cdot\mathbb{D}_2Q_j^{k,\alpha}.\end{aligned}$$

For notational convenience, we define $\varDelta_j^{k,\alpha}$ to be

$$\varDelta_j^{k,\alpha} = \sum_{\rho=0}^{s} \overline{\varTheta}_j^{k,\alpha\rho} \cdot \bar{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} \overline{\varXi}_j^{k,\alpha\nu} \cdot \overline{\eta}_i^{k,\nu} + \overline{\xi}_j^{k,\alpha} \qquad \forall\alpha = 0,\, 1,\, \cdots,\, s-1. \quad \text{(D.22)}$$

such that Eq. (D.21) is rewritten as

$$\sum_{\gamma=1}^{s} \varLambda_j^{k,\alpha\gamma} \cdot \delta q_j^{k,\gamma} = -r_j^{k,\alpha} - \varDelta_j^{k,\alpha} \qquad \forall\alpha = 0,\, 1,\, \cdots,\, s-1. \quad \text{(D.23)}$$

In addition, if we further define $\varLambda_j^k$, r_j^k, $\varDelta_j^k$ and $\delta\overline{q}_j^k$ respectively as

$$\begin{aligned}
\varLambda_j^k &= \left[\varLambda_j^{k,\alpha\gamma}\right] \in \mathbb{R}^{s\times s},\\
r_j^k &= \left[r_j^{k,0}\; r_j^{k,1}\; \cdots\; r_j^{k,s-1}\right]^T \in \mathbb{R}^s,\\
\varDelta_j^k &= \left[\varDelta_j^{k,0}\; \varDelta_j^{k,1}\; \cdots\; \varDelta_j^{k,s-1}\right]^T \in \mathbb{R}^s,\\
\delta\overline{q}_j^k &= \left[\delta q_j^{k,1}\; \delta q_j^{k,2}\; \cdots\; \delta q_j^{k,s}\right]^T \in \mathbb{R}^s,
\end{aligned}$$

in which $0 \le \alpha \le s-1$ and $1 \le \gamma \le s$, then Eq. (D.23) is equivalent to requiring

$$\varLambda_j^k \cdot \delta\overline{q}_j^k = -r_j^k - \varDelta_j^k. \quad \text{(D.24)}$$

in which $\varLambda_j^k$ is invertible since $\mathcal{J}^{k^{-1}}(\overline{q}^k)$ exists. From Eq. (D.24), we obtain

$$\delta\overline{q}_j^k = -\varLambda_j^{k^{-1}}(r_j^k + \varDelta_j^k).$$

If $\varLambda_j^{k^{-1}}$ is explicitly written as $\varLambda_j^{k^{-1}} = \left[\overline{\varLambda}_j^{k,\gamma\varrho}\right] \in \mathbb{R}^{s\times s}$ in which $1 \le \gamma \le s$ and $0 \le \varrho \le s-1$, expanding the equation above, we obtain

$$\delta q_j^{k,\gamma} = -\sum_{\varrho=0}^{s-1} \overline{\varLambda}_j^{k,\gamma\varrho} \left(r_j^{k,\varrho} + \varDelta_j^{k,\varrho}\right) \qquad \forall\gamma = 1,\, 2,\, \cdots,\, s. \quad \text{(D.25)}$$

Substitute Eq. (D.22) into Eq. (D.25), the result is

$$\delta q_j^{k,\gamma} = \sum_{\rho=0}^{s} X_j^{k,\gamma\rho} \cdot \bar{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} Y_j^{k,\gamma\nu} \cdot \overline{\eta}_i^{k,\nu} + y_j^{k,\gamma} \quad \text{(D.26)}$$

in which

$$X_j^{k,\gamma\rho} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_j^{k,\gamma\varrho} \cdot \overline{\Theta}_j^{k,\varrho\rho},$$

$$Y_j^{k,\gamma\nu} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_j^{k,\gamma\varrho} \cdot \overline{\Xi}_j^{k,\varrho\nu},$$

$$y_j^{k,\gamma} = -\sum_{\varrho=0}^{s-1} \overline{\Lambda}_j^{k,\gamma\varrho} \left(r_j^{k,\varrho} + \overline{\xi}_j^{k,\varrho} \right).$$

Making use of Eqs. (D.18) and (D.26) and canceling out $\delta q_j^{k,\gamma}$, we obtain

$$\bar{\delta}\overline{\mu}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} \cdot \delta q_j^{k,\alpha} = \sum_{\rho=0}^{s} \overline{D}_j^{k,\rho} \cdot \bar{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} \overline{G}_j^{k,\alpha\nu} \cdot \overline{\eta}_i^{k,\nu} + \overline{l}_j^{k,\alpha} \tag{D.27}$$

in which $\alpha = 0,\ 1,\ \cdots,\ s$, and

$$\overline{D}_j^{k,\rho} = D_j^{k,\rho} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} X_j^{k,\gamma\rho} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} X_j^{k,\alpha\rho}, \tag{D.28a}$$

$$\overline{G}_j^{k,\nu} = G_j^{k,\alpha\nu} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} Y_j^{k,\gamma\nu} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} Y_j^{k,\alpha\nu}, \tag{D.28b}$$

$$\overline{l}_j^{k,\alpha} = l_j^{k,\alpha} + \sum_{\gamma=1}^{s} H_j^{k,\alpha\gamma} y_j^{k,\gamma} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\mu}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} y_j^{k,\alpha}, \tag{D.28c}$$

and note that $\overline{\sigma}^{\alpha 0}$ is given in Eq. (B.2) of Algorithm B.2. In a similar way, using Eqs. (D.19) and (D.26), we obtain

$$\bar{\delta}\overline{\Gamma}_j^{k,\alpha} - \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} \cdot \delta q_j^{k,\alpha} = \sum_{\rho=0}^{s} \overline{\Pi}_j^{k,\alpha\rho} \cdot \bar{\delta}\overline{v}_j^{k,\rho} + \sum_{\nu=1}^{s} \overline{\Psi}_j^{k,\alpha\nu} \cdot \overline{\eta}_j^{k,\nu} + \overline{\zeta}_j^{k,\alpha} \tag{D.29}$$

in which $\alpha = 1,\ 2,\ \cdots,\ s$, and

$$\overline{\Pi}_j^{k,\alpha\rho} = \Pi_j^{k,\alpha\rho} + \sum_{\gamma=1}^{s} \Phi_j^{k,\alpha\gamma} X_j^{k,\gamma\rho} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} X_j^{k,\alpha\rho}, \tag{D.30a}$$

$$\overline{\Psi}_j^{k,\alpha\nu} = \Psi_j^{k,\alpha\nu} + \sum_{\gamma=1}^{s} \Phi_j^{k,\alpha\gamma} Y_j^{k,\gamma\nu} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} Y_j^{k,\alpha\nu}, \tag{D.30b}$$

$$\overline{\zeta}_j^{k,\alpha} = \zeta_j^{k,\alpha} + \sum_{\gamma=1}^{s} \Phi_j^{k,\alpha\gamma} y_j^{k,\gamma} - \overline{\sigma}^{\alpha 0} \mathrm{ad}^D_{\overline{\Gamma}_j^{k,\alpha}} \overline{S}_j^{k,\alpha} y_j^{k,\alpha}. \tag{D.30c}$$

Finally, for each $j \in \mathrm{chd}(i)$, substituting Eqs. (D.27) and (D.29) respectively into Eqs. (D.12a) and (D.12b) and applying Eqs. (D.28) and (D.30) to expand $\overline{D}_j^{k,\rho}$, $\overline{G}_j^{k,\nu}$,

$\overline{l}_j^{k,\alpha}$ and $\overline{\Pi}_j^{k,\alpha\rho}$, $\overline{\Psi}_j^{k,\alpha\nu}$, $\overline{\zeta}_j^{k,\alpha}$, we respectively obtain $D_i^{k,\rho}$, $G_i^{k,\nu}$, $l_i^{k,\alpha}$ and $\Pi_i^{k,\alpha\rho}$, $\Psi_i^{k,\alpha\nu}$, $\zeta_i^{k,\alpha}$ as Eqs. (B.1) and (B.3) of Algorithm B.2 such that

$$\overline{\delta}\overline{\mu}_i^{k,\alpha} = \sum_{\rho=0}^{s} D_i^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} G_i^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu} + l_i^{k,\alpha} \qquad \forall\alpha = 0,\, 1,\, \cdots,\, s, \tag{D.31}$$

$$\overline{\delta}\overline{\Gamma}_i^{k,\alpha} = \sum_{\rho=0}^{s} \Pi_i^{k,\alpha\rho}\cdot\overline{\delta}\overline{v}_i^{k,\rho} + \sum_{\nu=1}^{s} \Psi_i^{k,\alpha\nu}\cdot\overline{\eta}_i^{k,\nu} + \zeta_i^{k,\alpha} \qquad \forall\alpha = 0,\, 1,\, \cdots,\, s-1. \tag{D.32}$$

In particular, note that even if rigid body i is the leaf node of the tree representation whose $\mathrm{chd}(i) = \emptyset$, there still exists $D_i^{k,\rho}$, $G_i^{k,\nu}$, $l_i^{k,\alpha}$ and $\Pi_i^{k,\alpha\rho}$, $\Psi_i^{k,\alpha\nu}$, $\zeta_i^{k,\alpha}$ from Eqs. (B.1) and (B.3) of Algorithm B.2. Moreover, as long as $D_i^{k,\rho}$, $G_i^{k,\nu}$, $l_i^{k,\alpha}$ and $\Pi_i^{k,\alpha\rho}$, $\Psi_i^{k,\alpha\nu}$, $\zeta_i^{k,\alpha}$ are given for each rigid body i, we can further obtain $X_i^{k,\alpha\rho}$, $Y_i^{k,\alpha\nu}$, $y_i^{k,\alpha}$ following lines 3 to 9 of Algorithm B.2.

In summary, for each rigid body i, we have shown that $X_i^{k,\alpha\rho}$, $Y_i^{k,\alpha\nu}$, $y_i^{k,\alpha}$ as well as $D_i^{k,\rho}$, $G_i^{k,\nu}$, $l_i^{k,\alpha}$ and $\Pi_i^{k,\alpha\rho}$, $\Psi_i^{k,\alpha\nu}$, $\zeta_i^{k,\alpha}$ are computable through the backward pass by Algorithm B.2, and $\delta q_i^{k,\alpha}$ as well as $\overline{\eta}_i^{k,\alpha}$ and $\overline{\delta}\overline{v}_i^{k,\alpha}$ are computable through the forward pass by lines 4 to 15 of Algorithm B.1, which proves the correctness of the algorithms.

In regard to the complexity, Algorithm B.2 has $O(s^2) + O(s^3)$ complexity since there are $O(s^2)$ quantities and the computation of $\Lambda_i^{k,\alpha^{-1}}$ takes $O(s^3)$ time, and thus the backward pass by lines 1 to 3 of Algorithm B.1 totally takes $O(s^3 n + s^2 n)$ time. Moreover, in lines 4 to 15 of Algorithm B.1, the forward pass takes $O(s^2 n)$ time. As a result, the overall complexity of Algorithm B.1 is $O(s^3 n)$, which proves the complexity of the algorithms. □

D.3 Proof of Proposition 3

Proposition 3. *For the kinetic energy $K(q, \dot{q})$ of a mechanical system, $\frac{\partial^2 K}{\partial \dot{q}^2}$, $\frac{\partial^2 K}{\partial \dot{q}\partial q}$, $\frac{\partial^2 K}{\partial q\partial \dot{q}}$, $\frac{\partial^2 K}{\partial q^2}$ can be recursively computed with Algorithm 2 in $O(n^2)$ time.*

Proof. According to Eqs. (D.1), (D.8) and (D.9), we have

$$\frac{\partial K}{\partial \dot{q}_i} = \overline{S}_i^T\Big(\overline{M}_i\overline{v}_i + \sum_{i'\in\mathrm{des}(i)} \overline{M}_{i'}\overline{v}_{i'}\Big) \tag{D.33}$$

and

$$\frac{\partial K}{\partial q_i} = \dot{\overline{S}}_i^T\Big(\overline{M}_i\overline{v}_i + \sum_{i'\in\mathrm{des}(i)} \overline{M}_{i'}\overline{v}_{i'}\Big). \tag{D.34}$$

Since $\overline{M}_i\overline{v}_i$, $\overline{S}_i$ and $\dot{\overline{S}}_i$ only depend on q_j and $\dot{q}_j$ for $j \in \mathrm{anc}(i) \cup \{i\}$, it is straightforward to show from Eqs. (D.33) and (D.34) that the derivatives $\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j}$, $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$, $\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j}$ and $\frac{\partial^2 K}{\partial q_i \partial q_j}$ can be respectively computed as

$$\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j} = \begin{cases} \frac{\partial}{\partial \dot{q}_j}\left(\frac{\partial K}{\partial \dot{q}_i}\right) & j \in \mathrm{anc}(i) \cup \{i\}, \\ \frac{\partial^2 K}{\partial \dot{q}_j \partial \dot{q}_i} & j \in \mathrm{des}(i), \\ 0 & \text{otherwise}, \end{cases} \tag{D.35}$$

$$\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j} = \begin{cases} \frac{\partial}{\partial q_j}\left(\frac{\partial K}{\partial \dot{q}_i}\right) & j \in \mathrm{anc}(i) \cup \{i\}, \\ \frac{\partial^2 K}{\partial q_j \partial \dot{q}_i} & j \in \mathrm{des}(i), \\ 0 & \text{otherwise}, \end{cases} \tag{D.36}$$

$$\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j} = \begin{cases} \frac{\partial}{\partial \dot{q}_j}\left(\frac{\partial K}{\partial q_i}\right) & j \in \mathrm{anc}(i) \cup \{i\}, \\ \frac{\partial^2 K}{\partial \dot{q}_j \partial q_i} & j \in \mathrm{des}(i), \\ 0 & \text{otherwise}, \end{cases} \tag{D.37}$$

$$\frac{\partial^2 K}{\partial q_i \partial q_j} = \begin{cases} \frac{\partial}{\partial q_j}\left(\frac{\partial K}{\partial q_i}\right) & j \in \mathrm{anc}(i) \cup \{i\}, \\ \frac{\partial^2 K}{\partial q_j \partial q_i} & j \in \mathrm{des}(i), \\ 0 & \text{otherwise}. \end{cases} \tag{D.38}$$

Therefore, we only need to consider the derivatives for $j \in \mathrm{anc}(i) \cup \{i\}$, whereas the derivatives for $j \notin \mathrm{anc}(i) \cup \{i\}$ are computed from Eqs. (D.35) to (D.38). In addition, if $j \in \mathrm{anc}(i) \cup \{i\}$, using Eqs. (C.14a), (C.10a), (C.11) and (C.12), we obtain

$$\frac{\partial \overline{M}_i\overline{v}_i}{\partial \dot{q}_j} = \overline{M}_i\overline{S}_j, \tag{D.39}$$

$$\begin{aligned} \frac{\partial \overline{M}_i\overline{v}_i}{\partial q_j} &= -\mathrm{ad}^T_{\overline{S}_j}\overline{M}_i\overline{v}_i - \overline{M}_i\mathrm{ad}_{\overline{S}_j}\overline{v}_i + \overline{M}_i\mathrm{ad}_{\overline{S}_j}(\overline{v}_i - \overline{v}_j) \\ &= \overline{M}_i\dot{\overline{S}}_j - \mathrm{ad}^T_{\overline{S}_j}\overline{M}_i\overline{v}_i \end{aligned} \tag{D.40}$$

$$\frac{\partial \dot{S}_i}{\partial \dot{q}_j} = \mathrm{ad}_{\overline{S}_j}\overline{S}_i, \tag{D.41}$$

$$\frac{\partial \dot{S}_i}{\partial q_j} = \mathrm{ad}_{\overline{v}_i}\mathrm{ad}_{\overline{S}_j}\overline{S}_i + \mathrm{ad}_{\mathrm{ad}_{\overline{S}_j}(\overline{v}_i - \overline{v}_j)}\overline{S}_i. \tag{D.42}$$

For notational clarity, we define $\overline{\mu}_i$, $\overline{\mathcal{M}}_i$, $\overline{\mathcal{M}}_i^A$ and $\overline{\mathcal{M}}_i^B$ as

$$\overline{\mu}_i = \overline{M}_i\overline{v}_i + \sum_{j \in \mathrm{des}(i)} \overline{M}_j\overline{v}_j = \overline{M}_i\overline{v}_i + \sum_{j \in \mathrm{chd}(i)} \overline{\mu}_j, \tag{D.43}$$

$$\overline{\mathcal{M}}_i = \overline{M}_i + \sum_{j\in \mathrm{des}(i)} \overline{M}_j = \overline{M}_i + \sum_{j\in \mathrm{chd}(i)} \overline{\mathcal{M}}_j, \tag{D.44}$$

$$\overline{\mathcal{M}}_i^A = \overline{\mathcal{M}}_i \overline{S}_i, \tag{D.45}$$

$$\overline{\mathcal{M}}_i^B = \overline{\mathcal{M}}_i \dot{\overline{S}}_i - \mathrm{ad}^D_{\mu_i} \overline{S}_i \tag{D.46}$$

which will be used in the derivation of $\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j}$, $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$, $\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j}$ and $\frac{\partial^2 K}{\partial q_i \partial q_j}$.

1) $\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j}$

If $j \in \mathrm{anc}(i) \cup \{i\}$, from Eqs. (D.33), (D.39), (D.44) and (D.45), it is simple to show that

$$\begin{aligned}
\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j} &= \frac{\partial}{\partial \dot{q}_j}\left(\frac{\partial K}{\partial \dot{q}_i}\right) \\
&= \overline{S}_i^T \Big(\overline{M}_i \overline{S}_j + \sum_{i'\in \mathrm{des}(i)} \overline{M}_{i'} \overline{S}_j\Big) \\
&= \overline{S}_i^T \Big(\overline{M}_i + \sum_{i'\in \mathrm{des}(i)} \overline{M}_{i'}\Big) \overline{S}_j \\
&= \overline{S}_j^T \overline{\mathcal{M}}_i \overline{S}_i \\
&= \overline{S}_j^T \overline{\mathcal{M}}_i^A.
\end{aligned} \tag{D.47}$$

2) $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$

If $j \in \mathrm{anc}(i) \cup \{i\}$, using Eqs. (C.7a), (D.33), (D.40), (D.44) and (D.45), we obtain

$$\begin{aligned}
\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j} &= \frac{\partial}{\partial q_j}\left(\frac{\partial K}{\partial \dot{q}_i}\right) \\
&= \sum_{i'\in \mathrm{des}(i)\cup\{i\}} \Big(\overline{S}_i^T \overline{M}_{i'} \dot{\overline{S}}_j - \overline{S}_i^T \mathrm{ad}^T_{\overline{S}_j} \overline{M}_{i'} \overline{v}_{i'} + \overline{S}_i^T \mathrm{ad}^T_{\overline{S}_j} \overline{M}_{i'} \overline{v}_{i'}\Big) \\
&= \overline{S}_i^T \Big(\overline{M}_i + \sum_{i'\in \mathrm{des}(i)} \overline{M}_{i'}\Big) \dot{\overline{S}}_j \\
&= \dot{\overline{S}}_j^T \overline{\mathcal{M}}_i \overline{S}_i \\
&= \dot{\overline{S}}_j^T \overline{\mathcal{M}}_i^A.
\end{aligned} \tag{D.48}$$

3) $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$

If $j \in \mathrm{anc}(i) \cup \{i\}$, using Eqs. (D.34), (D.39), (D.41), (D.43) and (D.44), we obtain

$$\begin{aligned}
\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j} &= \frac{\partial}{\partial \dot{q}_j}\left(\frac{\partial K}{\partial q_i}\right) \\
&= \sum_{i' \in \mathrm{des}(i)\cup\{i\}} \left(\dot{\overline{S}}_i^T \overline{M}_{i'} \overline{S}_j + \overline{S}_i^T \mathrm{ad}_{\overline{S}_j}^T \overline{M}_{i'} \overline{v}_{i'}\right) \\
&= \overline{S}_j^T \Big(\overline{M}_i + \sum_{i' \in \mathrm{des}(i)} \overline{M}_{i'}\Big)\dot{\overline{S}}_i + \Big(\overline{M}_i \overline{v}_i + \sum_{i' \in \mathrm{des}(i)} \overline{M}_{i'} \overline{v}_{i'}\Big)^T \mathrm{ad}_{\overline{S}_j} \overline{S}_i \\
&= \overline{S}_j^T \overline{\mathcal{M}}_i \dot{\overline{S}}_i + \overline{\mu}_i^T \mathrm{ad}_{\overline{S}_j} \overline{S}_i.
\end{aligned}$$

Then simplify the equation above with $\overline{\mu}_i^T \mathrm{ad}_{\overline{S}_j} \overline{S}_i = -\overline{S}_j^T \mathrm{ad}_{\overline{\mu}_i}^D \overline{S}_i$ and Eq. (D.46), the result is

$$\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j} = \overline{S}_j^T \left(\overline{\mathcal{M}}_i \dot{\overline{S}}_i - \mathrm{ad}_{\overline{\mu}_i}^D \overline{S}_i\right) = \overline{S}_j^T \overline{\mathcal{M}}_i^B. \tag{D.49}$$

4) $\frac{\partial^2 K}{\partial q_i \partial q_j}$

If $j \in \mathrm{anc}(i) \cup \{i\}$, using Eqs. (C.12), (D.34), (D.39), (D.40) and (D.42) to (D.44) and $\mathrm{ad}_{\mathrm{ad}_{\overline{v}_i}\overline{S}_j} = \mathrm{ad}_{\overline{v}_i}\mathrm{ad}_{\overline{S}_j} - \mathrm{ad}_{\overline{S}_j}\mathrm{ad}_{\overline{v}_i}$, we obtain

$$\begin{aligned}
\frac{\partial^2 K}{\partial q_i \partial q_j} &= \frac{\partial}{\partial q_j}\left(\frac{\partial K}{\partial q_i}\right) \\
&= \sum_{i' \in \mathrm{des}(i)\cup\{i\}} \Bigg[\left(\overline{M}_{i'} \overline{v}_{i'}\right)^T \Big(\mathrm{ad}_{\overline{v}_i}\mathrm{ad}_{\overline{S}_j} \overline{S}_i - \mathrm{ad}_{\overline{S}_j}\mathrm{ad}_{\overline{v}_i} \overline{S}_i + \\
&\qquad \mathrm{ad}_{\mathrm{ad}_{\overline{S}_j}(\overline{v}_i - \overline{v}_j)} \overline{S}_i\Big) + \dot{\overline{S}}_j^T \overline{M}_{i'} \dot{\overline{S}}_i \Bigg] \\
&= \dot{\overline{S}}_j^T \Big(\overline{M}_i + \sum_{i' \in \mathrm{des}(i)} \overline{M}_{i'}\Big)\dot{\overline{S}}_i + \Big(\overline{M}_i \overline{v}_i + \sum_{i' \in \mathrm{des}(i)} \overline{M}_{i'} \overline{v}_{i'}\Big)^T \mathrm{ad}_{\dot{\overline{S}}_j} \overline{S}_i \\
&= \dot{\overline{S}}_j^T \overline{\mathcal{M}}_i \dot{\overline{S}}_i + \overline{\mu}_i^T \mathrm{ad}_{\dot{\overline{S}}_j} \overline{S}_i.
\end{aligned}$$

Similar to $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$, using $\overline{\mu}_i^T \mathrm{ad}_{\dot{\overline{S}}_j} \overline{S}_i = -\dot{\overline{S}}_j^T \mathrm{ad}_{\overline{\mu}_i}^D \overline{S}_i$ and Eq. (D.46), we obtain

$$\frac{\partial^2 K}{\partial q_i \partial q_j} = \dot{\overline{S}}_j^T \left(\overline{\mathcal{M}}_i \dot{\overline{S}}_i - \mathrm{ad}_{\overline{\mu}_i}^D \overline{S}_i\right) = \dot{\overline{S}}_j^T \overline{\mathcal{M}}_i^B. \tag{D.50}$$

Thus far, we have proved that $\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j}$, $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$, $\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j}$ and $\frac{\partial^2 K}{\partial q_i \partial q_j}$ can be computed using Eqs. (D.35) to (D.38) and (D.47) to (D.50) with which we further have $\frac{\partial^2 K}{\partial \dot{q}^2}$, $\frac{\partial^2 K}{\partial \dot{q} \partial q}$, $\frac{\partial^2 K}{\partial q \partial \dot{q}}$ and $\frac{\partial^2 K}{\partial q^2}$ computed.

As for the complexity of Algorithm 2, it takes $O(n)$ time to pass the tree representation forward to compute g_i, M_i, $\overline{S}_i$, $\overline{v}_i$, $\dot{\overline{S}}_i$ and another $O(n)$ time to pass the tree representation backward to compute $\overline{\mu}_i$, $\overline{\mathcal{M}}_i$, $\overline{\mathcal{M}}_i^A$ and $\overline{\mathcal{M}}_i^B$. In the backward pass, $\frac{\partial^2 K}{\partial \dot{q}_i \partial \dot{q}_j}$, $\frac{\partial^2 K}{\partial \dot{q}_i \partial q_j}$, $\frac{\partial^2 K}{\partial q_i \partial \dot{q}_j}$ and $\frac{\partial^2 K}{\partial q_i \partial q_j}$ are computed for each i using Eqs. (D.35) to (D.38) and (D.47) to (D.50) which totally takes at most $O(n^2)$ time. Therefore, the complexity of Algorithm 2 is $O(n^2)$. This completes the proof. □

D.4 Proof of Proposition 4

Proposition 4. *If* $\mathbf{g} \in \mathbb{R}^3$ *is gravity, then for the gravitational potential energy* $V_{\mathbf{g}}(q)$*,* $\frac{\partial^2 V_{\mathbf{g}}}{\partial q^2}$ *can be recursively computed with Algorithm 3 in* $O(n^2)$ *time.*

Proof. It is known that the gravitational potential energy $V_{\mathbf{g}}(q)$ is

$$V_{\mathbf{g}}(q) = -\sum_{i=1}^{n} m_i \cdot \mathbf{g}^T p_i. \tag{D.51}$$

in which $m_i \in \mathbb{R}$ is the mass of rigid body i and $p_i \in \mathbb{R}^3$ is the mass center of rigid body i as well as the origin of frame $\{i\}$. In addition, from Eqs. (C.5a) and (C.5b), we have

$$\frac{\partial p_i}{\partial q_j} = \begin{cases} \hat{\overline{s}}_j p_i + \overline{n}_j & j \in \text{anc}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{D.52a}$$

and

$$\frac{\partial p_j}{\partial q_i} = \begin{cases} \hat{\overline{s}}_i p_j + \overline{n}_i & j \in \text{des}(i) \cup \{i\}, \\ 0 & \text{otherwise}, \end{cases} \tag{D.52b}$$

in which $\overline{s}_i, \overline{n}_i \in \mathbb{R}^3$ and $\overline{S}_i = \begin{bmatrix} \overline{s}_i^T & \overline{n}_i^T \end{bmatrix}^T \in \mathbb{R}^6$ is the spatial Jacobian of joint i. From Eqs. (D.52b) and (D.51), algebraic manipulation gives

$$\frac{\partial V_{\mathbf{g}}}{\partial q_i} = -\overline{S}_i^T \left(m_i \begin{bmatrix} \hat{p}_i \mathbf{g} \\ \mathbf{g} \end{bmatrix} + \sum_{i' \in \text{des}(i)} m_{i'} \begin{bmatrix} \hat{p}_{i'} \mathbf{g} \\ \mathbf{g} \end{bmatrix} \right). \tag{D.53}$$

Moreover, observe that $\overline{S}_i$ and p_i only depends on q_j for $j \in \text{anc}(i) \cup \{i\}$, we obtain from Eq. (D.53) that

$$\frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j} = \begin{cases} \frac{\partial}{\partial q_j} \left(\frac{\partial V_{\mathbf{g}}}{\partial q_i} \right) & j \in \text{anc}(i) \cup \{i\}, \\ \frac{\partial^2 V_{\mathbf{g}}}{\partial q_j \partial q_i} & j \in \text{des}(i), \\ 0 & \text{otherwise}, \end{cases} \tag{D.54}$$

which means that only $\frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j}$ for $j \in \text{anc}(i) \cup \{i\}$ needs to be explicitly computed. If $j \in \text{anc}(i) \cup \{i\}$, using Eqs. (C.7a), (D.52a) and (D.53) as well as the equality $\hat{a}b = -\hat{b}a$ for any $a, b \in \mathbb{R}^3$, we obtain

$$\begin{aligned} \frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j} &= \frac{\partial}{\partial q_j} \left(\frac{\partial V_{\mathbf{g}}}{\partial q_i} \right) \\ &= \sum_{i' \in \text{des}(i) \cup \{i\}} m_{i'} \left[\overline{s}_i^T \left(\hat{\mathbf{g}} \hat{\overline{s}}_j p_{i'} + \hat{\overline{s}}_j \hat{p}_{i'} \mathbf{g} \right) - \overline{n}_i^T \hat{\mathbf{g}} \overline{s}_j \right]. \end{aligned}$$

In addition, since $\hat{p}_{i'}\hat{\mathbf{g}}\overline{s}_j = -\hat{\mathbf{g}}\hat{\overline{s}}_j p_{i'} - \hat{\overline{s}}_j \hat{p_{i'}}\mathbf{g}$ and $\hat{a}^T = -\hat{a}$ for any $a \in \mathbb{R}^3$, the equation above is equivalent to

$$\frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j} = \overline{s}_j^T \hat{\mathbf{g}} \Big[\big(m_i + \sum_{i' \in \mathrm{des}(i)} m_{i'} \big) \overline{n}_i - \big(m_i \hat{p}_i + \sum_{i' \in \mathrm{des}(i)} m_{i'} \hat{p}_{i'} \big) \overline{s}_i \Big] \tag{D.55}$$

If we define

$$\overline{\sigma}_{m_i} = m_i + \sum_{j \in \mathrm{des}(i)} m_j = m_i + \sum_{j \in \mathrm{chd}(i)} \overline{\sigma}_{m_j},$$

$$\overline{\sigma}_{p_i} = m_i p_i + \sum_{j \in \mathrm{des}(i)} m_j p_j = m_i p_i + \sum_{j \in \mathrm{chd}(i)} \overline{\sigma}_{p_j},$$

$$\overline{\sigma}_i^A = \hat{\mathbf{g}} \left(\overline{\sigma}_{m_i} \cdot \overline{n}_i - \hat{\overline{\sigma}}_{p_i} \cdot \overline{s}_i \right),$$

then Eq. (D.55) is further simplified to

$$\frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j} = \overline{s}_j^T \hat{\mathbf{g}} \left(\overline{\sigma}_{m_i} \overline{n}_i - \hat{\overline{\sigma}}_{p_i} \overline{s}_i \right) = \overline{s}_j^T \overline{\sigma}_i^A. \tag{D.56}$$

As a result, $\frac{\partial^2 V_{\mathbf{g}}}{\partial q^2}$ can be computed from Eqs. (D.54) and (D.56).

The $O(n^2)$ complexity of Algorithm 3 is as follows: the forward pass to compute g_i and $\overline{S}_i$ and the backward pass to compute $\overline{\sigma}_{m_i}$, $\overline{\sigma}_{p_i}$ and $\overline{\sigma}_i^A$ take $O(n)$ time, respectively; and the computation of $\frac{\partial^2 V_{\mathbf{g}}}{\partial q_i \partial q_j} = \frac{\partial^2 V_{\mathbf{g}}}{\partial q_j \partial q_i} = \overline{s}_j^T \overline{\sigma}_i^A$ totally takes $O(n^2)$ time. Therefore, it can be concluded that Algorithm 3 has $O(n^2)$ complexity. This completes the proof. □

References

1. Taosha Fan, Jarvis Schultz, and Todd D Murphey. Efficient computation of variational integrators in robotic simulation and trajectory optimization. In *International Workshop on the Algorithmic Foundations of Robotics (WAFR)*, 2018.