Physics Simulation Cookbook

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Abstract

This cookbook provides a curated collection of fundamental equations essential for simulating solid bodies.

Keywords Physics simulation

Contents

1 Lagrangian Mechanics

1.1 States

$\boldsymbol{q} = \boldsymbol{q}(t)$ is the generalized coordinates (= position in Cartesian coordinates).

$\dot{\boldsymbol{q}} = \dot{\boldsymbol{q}}(t)$ is the generalized velocity (= velocity in Cartesian coordinates), i.e. the time derivative of the generalized coordinates.

$$\dot{\boldsymbol{q}}(t) = \frac{d\boldsymbol{q}}{dt} \tag{1}$$

$\ddot{\boldsymbol{q}} = \ddot{\boldsymbol{q}}(t)$ is the generalized acceleration (= acceleration in Cartesian coordinates), i.e. the time derivative of the generalized velocity.

$$\ddot{\boldsymbol{q}}(t) = \frac{d\dot{\boldsymbol{q}}}{dt} = \frac{d^2\boldsymbol{q}}{dt^2} \tag{2}$$

If we combine Equation 1 and Equation 2:

$$\begin{bmatrix} \dot{\boldsymbol{q}}(t) \\ \ddot{\boldsymbol{q}}(t) \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} \boldsymbol{q}(t) \\ \dot{\boldsymbol{q}}(t) \end{bmatrix} \tag{3}$$

Global state

$$\boldsymbol{x}_{\boldsymbol{q}}(t) = \begin{bmatrix} \boldsymbol{q}(t) \\ \dot{\boldsymbol{q}}(t) \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} \dot{\boldsymbol{q}}(t) \\ \ddot{\boldsymbol{q}}(t) \end{bmatrix} = \frac{d\boldsymbol{x}_{\boldsymbol{q}}}{dt} \tag{5}$$

1.2 Kinetic Energy

The continuous total kinetic energy T of a deformable body with mass density $\rho(\boldsymbol{q})$ is given by integrating over the entire volume V:

$$\begin{aligned} \mathcal{T} &= \frac{1}{2} \int_V \|\dot{\boldsymbol{q}}(t)\|^2 \ \rho(\boldsymbol{q}) \ dv \\ &= \frac{1}{2} \int_V \dot{\boldsymbol{q}}(t)^T \cdot \dot{\boldsymbol{q}}(t) \ \rho(\boldsymbol{q}) \ dv \\ &= \frac{1}{2} \dot{\boldsymbol{q}}(t)^T \left(\int_V \rho(\boldsymbol{q}) dv \right) \dot{\boldsymbol{q}}(t) \end{aligned} \tag{6}$$

The term $\int_V \rho(\boldsymbol{q}) dv$ is called mass:

$$\boldsymbol{\mathcal{M}}(\boldsymbol{q}) = \int_V \rho(\boldsymbol{q}) dv \tag{7}$$

Therefore,

$$\mathcal{T} = \frac{1}{2} \ \dot{\boldsymbol{q}}(t)^T \ \boldsymbol{\mathcal{M}}(\boldsymbol{q}) \ \dot{\boldsymbol{q}}(t) \tag{8}$$

In general, the mass $\boldsymbol{\mathcal{M}}$ depends on the state $\boldsymbol{q}$, and therefore varies with time.

1.3 Lagrangian

The Lagrangian $\mathcal{L}$ of a system is defined as:

$$\mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \mathcal{T} - V \tag{9}$$

where:
- $\mathcal{T}$ is the total kinetic energy
- V is the potential energy

1.4 Forces

Conservative forces $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ are forces deriving from a potential energy:

$$\boldsymbol{F} = -\frac{\partial V}{\partial \boldsymbol{q}} \tag{10}$$

$\boldsymbol{\mathcal{K}}(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}}$ is called stiffness.

$\boldsymbol{\mathcal{B}}(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \frac{\partial \boldsymbol{F}}{\partial \dot{\boldsymbol{q}}}$ is called damping.

1.5 Momentum

The conjugate momentum is defined as:

$$\boldsymbol{p} = \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \tag{11}$$

Based on the definition of the Lagrangian (Equation 9):

$$\boldsymbol{p} = \frac{\partial \mathcal{T}}{\partial \dot{\boldsymbol{q}}} - \frac{\partial V}{\partial \dot{\boldsymbol{q}}} \tag{12}$$

When the potential energy does not depend on the velocity (magnetic forces, dissipative forces…):

$$\frac{\partial V}{\partial \dot{\boldsymbol{q}}} = 0 \tag{13}$$

Therefore,

$$\boldsymbol{p} = \frac{\partial \mathcal{T}}{\partial \dot{\boldsymbol{q}}} = \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ \dot{\boldsymbol{q}}(t) \tag{14}$$

1.6 Action

The action is the accumulation of values of the Lagrangian between two states:

$$S = \int_{t_1}^{t_2} \mathcal{L}\ dt \tag{15}$$

The action principles state that the true path of $\boldsymbol{q}$ from t_1 to t_2 is a stationary point of the action:

$$\delta S = \frac{dS}{d\boldsymbol{q}} = 0 \tag{16}$$

where δ represents a small variation of the trajectory.

1.7 Euler-Lagrange Equation

We develop the Lagrangian at the first-order:

$$\mathcal{L}(\boldsymbol{q} + \delta\boldsymbol{q}, \dot{\boldsymbol{q}} + \delta\dot{\boldsymbol{q}}, t) \approx \mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) + \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q} + \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}} \tag{17}$$

The variation of the action in terms of the first-order development:

$$
\begin{aligned}
\delta S &= S[\boldsymbol{q}+\delta\boldsymbol{q}] - S[\boldsymbol{q}] \\
&= \int_{t_1}^{t_2} \left(\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}},t) + \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q} + \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}} \right) dt - \int_{t_1}^{t_2} \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}},t)\; dt \\
&= \int_{t_1}^{t_2} \left[\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q} + \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}} \right] dt \\
&= \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q}\; dt + \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}}\; dt
\end{aligned}
\tag{18}
$$

The velocity term is transformed using integration by parts (Equation 322):

$$
\int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}}\; dt = \left[\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\boldsymbol{q} \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \right) \delta\boldsymbol{q}\; dt \tag{19}
$$

The position at t_1 and t_2 is fixed. Only the path from t_1 to t_2 is subject to change. It means that $\delta\boldsymbol{q}(t_1) = 0$ and $\delta\boldsymbol{q}(t_2) = 0$. We can deduce that $\left[\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\boldsymbol{q}\right]_{t_1}^{t_2} = 0$.

Finally, the velocity term is replaced in Equation 18:

$$
\begin{aligned}
\delta S &= \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q}\; dt + \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\delta\dot{\boldsymbol{q}}\; dt \\
&= \int_{t_1}^{t_2} \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q}\; dt - \int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \right) \delta\boldsymbol{q}\; dt \\
&= \int_{t_1}^{t_2} \left[\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}\delta\boldsymbol{q} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \right) \delta\boldsymbol{q} \right] dt \\
&= \int_{t_1}^{t_2} \left[\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \right) \right] \delta\boldsymbol{q}\; dt
\end{aligned}
\tag{20}
$$

From the fundamental lemma of the calculus of variations:

$$
\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} \right) = 0 \tag{21}
$$

This is the Euler-Lagrange equation.

2 Newton's Second Law of Motion

2.1 Deduction from the Lagrangian

We apply the Euler-Lagrange equation on the Lagrangian defined in Equation 9. It requires to compute $\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}$ and $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\right)$.

First, let's compute the term $\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}}$:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} = \frac{\partial \mathcal{T}}{\partial \boldsymbol{q}} - \frac{\partial V}{\partial \boldsymbol{q}} \tag{22}$$

$$\begin{aligned} \frac{\partial \mathcal{T}}{\partial \boldsymbol{q}} &= \frac{\partial}{\partial \boldsymbol{q}}\left[\frac{1}{2}\dot{\boldsymbol{q}}(t)^T \boldsymbol{\mathcal{M}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t)\right] \\ &= \frac{1}{2}\dot{\boldsymbol{q}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}}(t) \end{aligned} \tag{23}$$

Therefore,

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} = \frac{1}{2}\dot{\boldsymbol{q}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}}(t) + \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{24}$$

Then, the term $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\right)$ is the time derivative of the momentum (Equation 11):

$$\frac{d\boldsymbol{p}}{dt} = \frac{d\boldsymbol{\mathcal{M}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t)}{dt} = \dot{\boldsymbol{\mathcal{M}}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t) + \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ddot{\boldsymbol{q}}(t) \tag{25}$$

Putting all together from Equation 21:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\right) = 0 &\Leftrightarrow \frac{1}{2}\dot{\boldsymbol{q}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}}(t) + \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - \left(\dot{\boldsymbol{\mathcal{M}}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t) + \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ddot{\boldsymbol{q}}(t)\right) = 0 \\ &\Leftrightarrow \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ddot{\boldsymbol{q}}(t) + \dot{\boldsymbol{\mathcal{M}}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t) - \frac{1}{2}\dot{\boldsymbol{q}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}}(t) = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{aligned} \tag{26}$$

Let's us define the Coriolis and centrifugal terms $\boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ such that

$$\boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}})\dot{\boldsymbol{q}}(t) = \dot{\boldsymbol{\mathcal{M}}}(\boldsymbol{q})\dot{\boldsymbol{q}}(t) - \frac{1}{2}\dot{\boldsymbol{q}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}}{\partial \boldsymbol{q}}\dot{\boldsymbol{q}}(t) \tag{27}$$

The final form of the second Newton's law deduced from the Lagrangian is:

$$\boldsymbol{\mathcal{M}}(\boldsymbol{q})\ddot{\boldsymbol{q}}(t) + \boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}})\dot{\boldsymbol{q}}(t) = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{28}$$

In the special case where the mass does not depend on the position, nor time, $\boldsymbol{\mathcal{C}} = 0$. Then the Newton's law of motion is:

$$\boldsymbol{\mathcal{M}}(\boldsymbol{q})\ddot{\boldsymbol{q}}(t) = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{29}$$

2.2 Ordinary Differential Equation

Equation 28 is a second-order differential equation. We transform it to a first-order.

Substituting Equation 2 into Equation 28:

$$\boldsymbol{\mathcal{M}}(\boldsymbol{q})\frac{d\dot{\boldsymbol{q}}}{dt} + \boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}})\dot{\boldsymbol{q}}(t) = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{30}$$

Combined with Equation 1, we have a first-order ordinary differential equation in $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$:

$$\begin{bmatrix} \frac{d\boldsymbol{q}}{dt} \\ \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ \frac{d\dot{\boldsymbol{q}}}{dt} + \boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}})\dot{\boldsymbol{q}}(t) \end{bmatrix} = \begin{bmatrix} \dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{bmatrix} \tag{31}$$

2.2.1 Rayleigh Damping

Rayleigh damping is defined as:

$$F_{\text{Rayleigh}} = \left(-\alpha \boldsymbol{\mathcal{M}} + \beta \underbrace{\frac{\partial \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}}}_{\boldsymbol{\mathcal{K}}(\boldsymbol{q}, \dot{\boldsymbol{q}})} \right) \dot{\boldsymbol{q}} \tag{32}$$

F_{Rayleigh} is added to the sum of forces in Equation 31:

$$\begin{bmatrix} \frac{d\boldsymbol{q}}{dt} \\ \boldsymbol{\mathcal{M}}(\boldsymbol{q}) \frac{d\dot{\boldsymbol{q}}}{dt} + \boldsymbol{\mathcal{C}}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \dot{\boldsymbol{q}}(t) \end{bmatrix} = \begin{bmatrix} \dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + (-\alpha \boldsymbol{\mathcal{M}} + \beta \boldsymbol{\mathcal{K}}) \dot{\boldsymbol{q}} \end{bmatrix} \tag{33}$$

3 Statics

The physical system does not experience any acceleration ($\ddot{\boldsymbol{q}} = 0$). $\ddot{\boldsymbol{q}} = 0$ does not necessarily imply $\dot{\boldsymbol{q}} = 0$. It means that $\dot{\boldsymbol{q}}$ is a constant. If this constant is nonzero, it is called dynamic equilibrium or steady motion. In this section, we consider $\dot{\boldsymbol{q}} = 0$. Second Newton's law (Equation 28) becomes:

$$\boldsymbol{F}(\boldsymbol{q}) = 0 \tag{34}$$

This is a non-linear equation. It is solved using Newton-Raphson method.

Solve for $\Delta \boldsymbol{q}^i = \boldsymbol{q}^{i+1} - \boldsymbol{q}^i$:

$$\left.\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}}\right|_{\boldsymbol{q}^i} \Delta \boldsymbol{q}^i = -\boldsymbol{F}(\boldsymbol{q}^i) \tag{35}$$

This is a linear system to be solved.

With $\boldsymbol{\mathcal{K}}^i = \left.\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}}\right|_{\boldsymbol{q}^i}$, we solve:

$$\boldsymbol{\mathcal{K}}^i \, \Delta \boldsymbol{q}^i = -\boldsymbol{F}(\boldsymbol{q}^i) \tag{36}$$

Then,

$$\boldsymbol{q}^{i+1} = \Delta \boldsymbol{q}^i + \boldsymbol{q}^i \tag{37}$$

4 Spring

4.1 Linear Spring

DEFINITION

Hooke's law:

$$F = kx \tag{38}$$

x is the amount by which the free end of the spring was displaced from its "relaxed" position.

Considering two points a and b, $x = \|b - a\|$, and the force is exerted along the direction $b - a$.

Then:

$$F_a = k\left(\|b - a\| - L_0\right)\frac{b - a}{\|b - a\|} \tag{39}$$

$$F_b = k\left(\|a - b\| - L_0\right)\frac{a - b}{\|a - b\|} = -F_a \tag{40}$$

where:

- k is the spring stiffness constant
- a The position vector of the first end of the spring
- b The position vector of the second end of the spring.
- $\|b - a\|$ is the distance between the two ends of the spring,
- L_0 is the rest length of the spring.

To compute the derivative of F_a and F_b, we define $\delta = \|b - a\|$

$$\begin{aligned} F_a &= k(\delta - L_0)\frac{b - a}{\delta} \\ &= k\left(1 - \frac{L_0}{\delta}\right)(b - a) \\ &= k\left(b - a - \frac{L_0}{\delta}(b - a)\right) \end{aligned} \tag{41}$$

$$\begin{aligned} \frac{\partial F_a}{\partial a} &= k\frac{\partial}{\partial a}\left(b - a - \frac{L_0}{\delta}(b - a)\right) \\ &= -k\left(I + L_0\frac{\partial}{\partial a}\left(\frac{b - a}{\delta}\right)\right) \end{aligned} \tag{42}$$

From Equation 315,

$$\frac{\partial}{\partial a}\left(\frac{b - a}{\delta}\right) = -\frac{1}{\delta}I + \frac{1}{\delta^3}(b - a) \otimes (b - a) \tag{43}$$

Finally,

$$
\begin{aligned}
\frac{\partial F_a}{\partial a} &= -k\Big(I + L_0\Big(-\frac{1}{\delta}I + \frac{1}{\delta^3}(b-a)\otimes(b-a)\Big)\Big) \\
&= -k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I + \frac{L_0}{\delta^3}(b-a)\otimes(b-a)\Big) \\
&= -k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I + \frac{L_0}{\delta}\widehat{b-a}\otimes\widehat{b-a}\Big)
\end{aligned} \tag{44}
$$

RESULT

$$
\frac{\partial F_a}{\partial a} = -k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I + \frac{L_0}{\delta}\widehat{b-a}\otimes\widehat{b-a}\Big) \tag{45}
$$

Similarly,

$$
\begin{aligned}
\frac{\partial F_a}{\partial b} &= k\frac{\partial}{\partial b}\Big(b - a - \frac{L_0}{\delta}(b-a)\Big) \\
&= k\Big(I - L_0\frac{\partial}{\partial b}\Big(\frac{b-a}{\delta}\Big)\Big)
\end{aligned} \tag{46}
$$

From Equation 314,

$$
\frac{\partial}{\partial b}\Big(\frac{b-a}{\delta}\Big) = \frac{1}{\delta}I - \frac{1}{\delta^3}(b-a)\otimes(b-a) \tag{47}
$$

Finally,

$$
\begin{aligned}
\frac{\partial F_a}{\partial b} &= k\Big(I - L_0\Big(\frac{1}{\delta}I - \frac{1}{\delta^3}(b-a)\otimes(b-a)\Big)\Big) \\
&= k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I - \frac{L_0}{\delta^3}(b-a)\otimes(b-a)\Big) \\
&= k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I - \frac{L_0}{\delta}\widehat{b-a}\otimes\widehat{b-a}\Big)
\end{aligned} \tag{48}
$$

RESULT

$$
\frac{\partial F_a}{\partial b} = k\Big(\Big(1 - \frac{L_0}{\delta}\Big)I - \frac{L_0}{\delta}\widehat{b-a}\otimes\widehat{b-a}\Big) \tag{49}
$$

4.2 Nonlinear Spring

$$
F = F(x) \tag{50}
$$

4.2.1 Quadratic Spring

DEFINITION

$$
F = kx^2 \tag{51}
$$

Considering two points a and b, $\delta = \|b - a\|$,

$$
\begin{aligned}
F_a &= k\left(\|b-a\| - L_0\right)^2 \frac{b-a}{\|b-a\|} \\
&= k(\delta - L_0)^2 \frac{b-a}{\delta}
\end{aligned}
\tag{52}
$$

$$
\begin{aligned}
F_b &= k\left(\|a-b\| - L_0\right)^2 \frac{a-b}{\|a-b\|} \\
&= -k(\delta - L_0)^2 \frac{b-a}{\delta} \\
&= -F_a
\end{aligned}
\tag{53}
$$

5 Numerical Integration

5.1 Definition

For any function $y = y(t)$, we call

$$y_n = y(t_n) \tag{54}$$

with

$$t_n = t_0 + n\,\Delta t \tag{55}$$

Numerical methods for ordinary ordinary differential equation approximate solutions to initial value problems of the form:

$$y' = f(t, y), \quad y(t_0) = y_0 \tag{56}$$

5.2 Linear Multistep Method

$$\begin{gathered} y_{n+s} + a_{s-1} y_{n+s-1} + a_{s-2} y_{n+s-2} + \ldots + a_0 y_n = \\ \Delta t (b_s f(t_{n+s}, y_{n+s}) + b_{s-1} f(t_{n+s-1}, y_{n+s-1}) + \ldots + b_0 f(t_n, y_n)) \end{gathered} \tag{57}$$

or

$$\sum_{j=0}^{s} a_j y_{n+j} = \Delta t \sum_{j=0}^{s} b_j f(t_{n+j}, y_{n+j}) \tag{58}$$

If $b_s = 0$, the method is called "explicit": it is possible to compute y_{n+s} directly. If $b_s \neq 0$, the method is called "implicit": the value of y_{n+s} depends on the value of $f(t_{n+s}, y_{n+s})$.

5.3 Backward Differentiation Formula

Given a set of $s+1$ nodes $\{t_n, t_{n+1}, \ldots, t_{n+s}\}$, the Lagrange basis for polynomials of degree $\leq s$ for those notes is the set of polynomials $\{l_0(t), l_1(t), \ldots, l_s(t)\}$:

$$l_j(t) = \prod_{\substack{0 \leq m \leq s \\ m \neq j}} \frac{t - t_{n+m}}{t_{n+j} - t_{n+m}} \tag{59}$$

The Lagrange interpolating polynomial for those nodes through the corresponding values $\{y_n, y_{n+1}, \ldots, y_{n+s}\}$ is the linear combination:

$$L(t) = \sum_{j=0}^{s} y_{n+j} l_j(t) \tag{60}$$

5.3.1 Derivative:

$$L'(t) = \sum_{j=0}^{s} y_{n+j} l_j'(t) \tag{61}$$

$$l_j'(t) = \sum_{\substack{i=0 \\ i \neq j}}^{s} \left[\frac{1}{t_{n+j} - t_{n+i}} \prod_{\substack{m=0 \\ m \neq (i,j)}} \frac{t - t_{n+m}}{t_{n+j} - t_{n+m}} \right] \tag{62}$$

5.3.2 Lagrange polynomials to solve an ODE

We approximate y' by L' in Equation 56:

$$\sum_{j=0}^{s} y_{n+j} l_j'(t) = f(t, y) \tag{63}$$

We want to find $y(t_{n+s})$, therefore

$$\sum_{j=0}^{s} y_{n+j} l_j'(t_{n+s}) = f(t_{n+s}, y_{n+s}) \tag{64}$$

$$\sum_{j=0}^{s} y_{n+j} \left(\sum_{\substack{i=0 \\ i\neq j}}^{s} \left[\frac{1}{t_{n+j} - t_{n+i}} \prod_{\substack{m=0 \\ m\neq(i,j)}} \frac{t_{n+s} - t_{n+m}}{t_{n+j} - t_{n+m}} \right] \right) = f(t_{n+s}, y_{n+s}) \tag{65}$$

5.3.3 Constant Step Size

$$t_{n+j} = t_n + j\,\Delta t \tag{66}$$

So, for all i, j

$$\begin{aligned} t_{n+j} - t_{n+i} &= t_n + j\,\Delta t - (t_n + i\,\Delta t) \\ &= (j-i)\Delta t \end{aligned} \tag{67}$$

$$\sum_{j=0}^{s} y_{n+j} \left(\sum_{\substack{i=0 \\ i\neq j}}^{s} \left[\frac{1}{j-i} \prod_{\substack{m=0 \\ m\neq(i,j)}} \frac{s-m}{j-m} \right] \right) = \Delta t\ f(t_{n+s}, y_{n+s}) \tag{68}$$

BDF1

For $s = 1$:

$j = 0$:

$$l_0'(t_{n+1}) = \sum_{\substack{i=0 \\ i\neq 0}}^{1} \left[\frac{1}{0-i} \prod_{\substack{m=0 \\ m\neq(i,0)}} \frac{1-m}{-m} \right] = \frac{1}{-1} \prod_{\substack{m=0 \\ m\neq(1,0)}} \frac{1-m}{-m} = -1 \tag{69}$$

$j = 1$:

$$l_1'(t_{n+1}) = \sum_{\substack{i=0 \\ i\neq 1}}^{1} \left[\frac{1}{1-i} \prod_{\substack{m=0 \\ m\neq(i,1)}} \frac{1-m}{1-m} \right] = \frac{1}{1} \prod_{\substack{m=0 \\ m\neq(0,1)}} \frac{1-m}{1-m} = 1 \tag{70}$$

Finally, for $s = 1$:

$$y_{n+1} - y_n = \Delta t\ f(t_{n+1}, y_{n+1}) \tag{71}$$

BDF2

For $s = 2$:

$j = 0$:

$$\begin{aligned} l_0'(t_{n+2}) &= \sum_{\substack{i=0 \\ i\neq 0}}^{2} \left[\frac{1}{-i} \prod_{\substack{m=0 \\ m\neq(i,0)}} \frac{2-m}{-m} \right] \\ &= \left(\frac{1}{-1} \prod_{\substack{m=0 \\ m\neq(1,0)}} \frac{2-m}{-m} \right) + \left(\frac{1}{-2} \prod_{\substack{m=0 \\ m\neq(2,0)}} \frac{2-m}{-m} \right) \\ &= -\frac{1}{2}\left(\frac{2-1}{-1}\right) = \frac{1}{2} \end{aligned} \tag{72}$$

$j = 1$:

$$
\begin{aligned}
l_1'(t_{n+2}) &= \sum_{\substack{i=0\\ i\neq 1}}^{2}\left[\frac{1}{1-i}\prod_{\substack{m=0\\ m\neq(i,1)}}\frac{2-m}{1-m}\right]\\
&= \left(\frac{1}{1}\prod_{\substack{m=0\\ m\neq(0,1)}}\frac{2-m}{1-m}\right)+\left(\frac{1}{1-2}\prod_{\substack{m=0\\ m\neq(2,1)}}\frac{2-m}{1-m}\right)\\
&= -2
\end{aligned}
\tag{73}
$$

$j = 2$:

$$
\begin{aligned}
l_2'(t_{n+2}) &= \sum_{\substack{i=0\\ i\neq 2}}^{2}\left[\frac{1}{2-i}\prod_{\substack{m=0\\ m\neq(i,2)}}\frac{2-m}{2-m}\right]\\
&= \left(\frac{1}{2}\prod_{\substack{m=0\\ m\neq(0,2)}}\frac{2-m}{2-m}\right)+\left(\frac{1}{2-1}\prod_{\substack{m=0\\ m\neq(1,2)}}\frac{2-m}{2-m}\right)\\
&= \frac{3}{2}
\end{aligned}
\tag{74}
$$

Finally, for $s = 1$:

$$\frac{3}{2}y_{n+2} - 2y_{n+1} + \frac{1}{2}y_n = \Delta t\ f(t_{n+2}, y_{n+2}) \tag{75}$$

which can be written:

$$y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n = \frac{2}{3}\Delta t\ f(t_{n+2}, y_{n+2}) \tag{76}$$

5.4 Numerical Integration of Newton's Second Law of Motion

The second Newton's law (Equation 31) is a first-order ordinary differential equation of the form of Equation 56 ($y' = f(t, y), \quad y(t_0) = y_0$) where:

$$y(t) = \begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix} \tag{77}$$

$$f(t, y) = \begin{bmatrix}\dot{\boldsymbol{q}}(t)\\ \boldsymbol{\mathcal{M}}^{-1}(\boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - \boldsymbol{\mathcal{C}}\dot{\boldsymbol{q}})\end{bmatrix} \tag{78}$$

In case of Rayleigh damping (Equation 32):

$$f(t, y) = \begin{bmatrix}\dot{\boldsymbol{q}}(t)\\ \boldsymbol{\mathcal{M}}^{-1}(\boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - \boldsymbol{\mathcal{C}}\dot{\boldsymbol{q}} + (-\alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}}(\boldsymbol{q}, \dot{\boldsymbol{q}}))\dot{\boldsymbol{q}})\end{bmatrix} \tag{79}$$

5.5 Newton-Raphson

For implicit methods, Equation 58 is nonlinear. Newton-Raphson algorithm can be used to solve it.

5.5.1 Nonlinear function

Find the root x_r of a nonlinear function $r : \mathbb{R}^k \to \mathbb{R}^k$ such that:

$$r(x_r) = 0 \tag{80}$$

Let's define x^0 the first estimate of the solution of this equation, called the initial guess.

$$\Delta x^0 = x_r - x_0 \tag{81}$$

Taylor series expansion of r around x^0

$$\begin{aligned} r(x_r) &= r(x_0 + \Delta x_0) \\ &= r(x_0) + \left.\frac{\partial r}{\partial x}\right|_{x^0} \Delta x^0 + O\left(\left\|\Delta x^0\right\|^2\right) \end{aligned} \tag{82}$$

If we neglect second-order terms and higher:

$$r(x_r) \approx r(x_0) + \left.\frac{\partial r}{\partial x}\right|_{x^0} \Delta x^0 \tag{83}$$

If we use this approximation to solve the equation, it leads to:

$$r(x^0) + \left.\frac{\partial r}{\partial x}\right|_{x^0} \Delta x^0 = 0 \tag{84}$$

This is a linear system to solve for the unknown Δx^0:

$$\left.\frac{\partial r}{\partial x}\right|_{x^0} \Delta x^0 = -r(x^0) \tag{85}$$

Once Δx^0 is found, x^1 can be deduced:

$$x^1 = \Delta x^0 + x^0 \tag{86}$$

The process is repeated as

$$\left.\frac{\partial r}{\partial x}\right|_{x^i} (x^{i+1} - x^i) = -r(x^i) \tag{87}$$

6 Explicit Time Integration

6.1 Forward Euler Method

The time derivative in Equation 3 can be approximated using a forward first-order finite difference:

$$y'(t) \approx \frac{1}{\Delta t}(y(t+\Delta t) - y(t)) \Leftrightarrow \frac{d}{dt}\begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix} \approx \frac{1}{\Delta t}\left(\begin{bmatrix}\boldsymbol{q}(t+\Delta t)\\ \dot{\boldsymbol{q}}(t+\Delta t)\end{bmatrix} - \begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix}\right) \tag{88}$$

Substituting this approximation into Equation 31:

$$\frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}(t+\Delta t) - \boldsymbol{q}(t)\\ \boldsymbol{\mathcal{M}}(\boldsymbol{q})\ (\dot{\boldsymbol{q}}(t+\Delta t) - \dot{\boldsymbol{q}}(t))\end{bmatrix} = \begin{bmatrix}\dot{\boldsymbol{q}}(t)\\ \boldsymbol{F}(\boldsymbol{q},\dot{\boldsymbol{q}}) - \boldsymbol{\mathcal{C}}(\boldsymbol{q},\dot{\boldsymbol{q}})\dot{\boldsymbol{q}}(t)\end{bmatrix} \tag{89}$$

From Equation 54, we can also write:

$$\frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1} - \boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n)\end{bmatrix} = \begin{bmatrix}\dot{\boldsymbol{q}}_n\\ \boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n) - \boldsymbol{\mathcal{C}}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n\end{bmatrix} \tag{90}$$

Grouping the terms in $n+1$ on the left-hand side:

$$\begin{bmatrix}\boldsymbol{q}_{n+1}\\ \dot{\boldsymbol{q}}_{n+1}\end{bmatrix} = \begin{bmatrix}\boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}_n\\ \dot{\boldsymbol{q}}_n + \Delta t\ \boldsymbol{\mathcal{M}}^{-1}(\boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n) - \boldsymbol{\mathcal{C}}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n)\end{bmatrix} \tag{91}$$

6.2 Semi-implicit Euler method

The time derivative in Equation 3 can be approximated using a backward first-order finite difference for x and a forward first-order finite difference for v:

$$\frac{d}{dt}\begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix} \approx \frac{1}{\Delta t}\left(\begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t+\Delta t)\end{bmatrix} - \begin{bmatrix}\boldsymbol{q}(t-\Delta t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix}\right) \tag{92}$$

Substituting this approximation into Equation 3:

$$\begin{bmatrix}\dot{\boldsymbol{q}}(t)\\ \ddot{\boldsymbol{q}}(t)\end{bmatrix} = \frac{1}{\Delta t}\left(\begin{bmatrix}\boldsymbol{q}(t)\\ \dot{\boldsymbol{q}}(t+\Delta t)\end{bmatrix} - \begin{bmatrix}\boldsymbol{q}(t-\Delta t)\\ \dot{\boldsymbol{q}}(t)\end{bmatrix}\right) \tag{93}$$

From Equation 54, we can also write:

$$\begin{bmatrix}\dot{\boldsymbol{q}}_n\\ \ddot{\boldsymbol{q}}_n\end{bmatrix} = \frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_n - \boldsymbol{q}_{n-1}\\ \dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n\end{bmatrix} \tag{94}$$

or

$$\begin{bmatrix}\dot{\boldsymbol{q}}_{n+1}\\ \ddot{\boldsymbol{q}}_n\end{bmatrix} = \frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1} - \boldsymbol{q}_n\\ \dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n\end{bmatrix} \tag{95}$$

Multiplying the second line of Equation 95 by $\boldsymbol{\mathcal{M}}$:

$$\begin{bmatrix}\dot{\boldsymbol{q}}_{n+1}\\ \boldsymbol{\mathcal{M}}\ddot{\boldsymbol{q}}_n\end{bmatrix} = \frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1} - \boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n)\end{bmatrix} \tag{96}$$

From Equation 28:

$$\begin{bmatrix}\dot{\boldsymbol{q}}_{n+1}\\ \boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n) - \boldsymbol{\mathcal{C}}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n\end{bmatrix} = \frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1} - \boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n)\end{bmatrix} \tag{97}$$

Finally,

$$
\begin{bmatrix} \boldsymbol{q}_{n+1} \\ \dot{\boldsymbol{q}}_{n+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_n + \Delta t \ \dot{\boldsymbol{q}}_{n+1} \\ \dot{\boldsymbol{q}}_n + \Delta t \ \boldsymbol{\mathcal{M}}^{-1}(\boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) - \boldsymbol{\mathcal{C}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n) \end{bmatrix} \tag{98}
$$

7 Implicit Time Integration

7.1 Backward Differentiation Formula

A family of implicit methods for the numerical integration of ordinary differential equations

$$\sum_{k=0}^{s} \ddot{\boldsymbol{q}}_k y_{n+k} = \Delta t \; \beta \; f(t_{n+s}, y_{n+s}) \tag{99}$$

- For any $n \geq 0$, $t_n = t_0 + n \; \Delta t$
- y_n denotes the state at time t_n
- $\ddot{\boldsymbol{q}}_k$ and β are coefficients that depend on the order s of the method
- f the function of the ODE

Coefficients [1]:

Order	$\ddot{\boldsymbol{q}}_0$	$\ddot{\boldsymbol{q}}_1$	$\ddot{\boldsymbol{q}}_2$	$\ddot{\boldsymbol{q}}_3$	$\ddot{\boldsymbol{q}}_4$	$\ddot{\boldsymbol{q}}_5$	$\ddot{\boldsymbol{q}}_6$	β
1	-1	1						1
2	1	-4	3					2
3	-2	9	-18	11				6
4	3	-16	36	-48	25			12
5	-12	75	-200	300	-300	137		60
6	10	-72	225	-400	450	-360	147	60

7.2 1-step BDF (Backward Euler)

In Equation 56, the time derivative can be approximated using the backward first-order finite differences:

$$y'_{n+1} \approx \frac{y_{n+1} - y_n}{\Delta t} \Leftrightarrow \frac{d}{dt}\begin{bmatrix} \boldsymbol{q}(t+\Delta t) \\ \dot{\boldsymbol{q}}(t+\Delta t) \end{bmatrix} \approx \frac{1}{\Delta t}\left(\begin{bmatrix} \boldsymbol{q}(t+\Delta t) \\ \dot{\boldsymbol{q}}(t+\Delta t) \end{bmatrix} - \begin{bmatrix} \boldsymbol{q}(t) \\ \dot{\boldsymbol{q}}(t) \end{bmatrix}\right) \tag{100}$$

Equation 56 becomes:

$$\begin{aligned} \frac{y_{n+1} - y_n}{\Delta t} &= f(t + \Delta t, y_{n+1}) \\ \Leftrightarrow y_{n+1} - y_n &= \Delta t \; f(t + \Delta t, y_{n+1}) \end{aligned} \tag{101}$$

We observe that the method enters into the category of linear multistep methods (Equation 58) with:

$$\begin{cases} s &= 1 \\ a_1 &= 1 \\ a_0 &= -1 \\ b_1 &= 1 \\ b_0 &= 0 \end{cases} \tag{102}$$

We apply this equation on y from Equation 77 and f from Equation 78:

$$\begin{bmatrix} \boldsymbol{q}_{n+1} - \boldsymbol{q}_n \\ \dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n \end{bmatrix} = \Delta t \begin{bmatrix} \dot{\boldsymbol{q}}_{n+1} \\ \boldsymbol{\mathcal{M}}^{-1}\boldsymbol{F}(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) \end{bmatrix} \tag{103}$$

We multiply the second line by $\boldsymbol{\mathcal{M}}$ to get rid of the inverse:

$$\begin{bmatrix} \boldsymbol{q}_{n+1} - \boldsymbol{q}_n \\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n) \end{bmatrix} = \Delta t \begin{bmatrix} \dot{\boldsymbol{q}}_{n+1} \\ \boldsymbol{F}(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) \end{bmatrix} \tag{104}$$

This is a non-linear set of equations: $\boldsymbol{F}$ is non-linear with respect to the unknown $\boldsymbol{q}_{n+1}$ and $\dot{\boldsymbol{q}}_{n+1}$.

Let's define the residual function r such that:

$$r(\boldsymbol{x}_{\boldsymbol{q}}) = r(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \begin{bmatrix} \boldsymbol{q} - \boldsymbol{q}_n - \Delta t\ \dot{\boldsymbol{q}} \\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}} - \dot{\boldsymbol{q}}_n) - \Delta t\ F(\boldsymbol{x}_{\boldsymbol{q}}) \end{bmatrix} = \begin{bmatrix} r_1(\boldsymbol{x}_{\boldsymbol{q}}) \\ r_2(\boldsymbol{x}_{\boldsymbol{q}}) \end{bmatrix} \tag{105}$$

Based on Equation 104, we want to find the root $\boldsymbol{x}_{\boldsymbol{q}_{n+1}} = \begin{bmatrix} \boldsymbol{q}_{n+1} \\ \dot{\boldsymbol{q}}_{n+1} \end{bmatrix}$ of r such that

$$r\left(\boldsymbol{x}_{\boldsymbol{q}_{n+1}}\right) = 0 \tag{106}$$

We will need to compute the Jacobian J_r of r:

$$J_r = \frac{\partial r}{\partial x} = \begin{bmatrix} \frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} \\ \frac{\partial r_2}{\partial \boldsymbol{q}} & \frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} \end{bmatrix} \tag{107}$$

Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = I \tag{108}$$

$$\frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} = -\Delta t\ I \tag{109}$$

$$\frac{\partial r_2}{\partial \boldsymbol{q}} = -\Delta t\ \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}} = -\Delta t\ \boldsymbol{\mathcal{K}} \tag{110}$$

$$\frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} = \boldsymbol{\mathcal{M}} - \Delta t\ \frac{\partial \boldsymbol{F}}{\partial \dot{\boldsymbol{q}}} = \boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}} \tag{111}$$

The final expression of the Jacobian is:

$$J_r = \frac{\partial r}{\partial \boldsymbol{x}_{\boldsymbol{q}}} = \begin{bmatrix} \boldsymbol{I} & -\Delta t\ \boldsymbol{I} \\ -\Delta t\ \boldsymbol{\mathcal{K}} & \boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}} \end{bmatrix} \tag{112}$$

Let's define $\boldsymbol{q}^0$ and $\dot{\boldsymbol{q}}^0$ the first estimate of the solution of this equation, called the initial guess.

Newton-Raphson to solve $r(\boldsymbol{x}_{\boldsymbol{q}}) = 0$:

$$J_r({\boldsymbol{x}_{\boldsymbol{q}}}^i)({\boldsymbol{x}_{\boldsymbol{q}}}^{i+1} - {\boldsymbol{x}_{\boldsymbol{q}}}^i) = -r({\boldsymbol{x}_{\boldsymbol{q}}}^i) \tag{113}$$

$$\begin{bmatrix} \boldsymbol{I} & -\Delta t\ \boldsymbol{I} \\ -\Delta t\ \boldsymbol{\mathcal{K}}({\boldsymbol{x}_{\boldsymbol{q}}}^i) & \boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}({\boldsymbol{x}_{\boldsymbol{q}}}^i) \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \end{bmatrix} = \begin{bmatrix} -\boldsymbol{q}^i + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^i \\ -\boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^i - \dot{\boldsymbol{q}}_n) + \Delta t\ \boldsymbol{F}({\boldsymbol{x}_{\boldsymbol{q}}}^i) \end{bmatrix} \tag{114}$$

7.2.1 Solve for $\dot{\boldsymbol{q}}$

Using the Schur complement (see Equation 319), we obtain the reduced equation in $\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i$:

$$\begin{aligned} &\left(\boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}({\boldsymbol{x}_{\boldsymbol{q}}}^i) - \left(-\Delta t\ \boldsymbol{\mathcal{K}}({\boldsymbol{x}_{\boldsymbol{q}}}^i)\right)(-\Delta t\ \boldsymbol{I})\right)(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = \\ &-\boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^i - \dot{\boldsymbol{q}}_n) + \Delta t\ \boldsymbol{F}({\boldsymbol{x}_{\boldsymbol{q}}}^i) - \left(-\Delta t\ \boldsymbol{\mathcal{K}}({\boldsymbol{x}_{\boldsymbol{q}}}^i)\right)(-\boldsymbol{q}^i + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^i) \end{aligned} \tag{115}$$

Cleaning:

$$\begin{aligned} &\left(\boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}({\boldsymbol{x}_{\boldsymbol{q}}}^i) + \Delta t^2\ \boldsymbol{\mathcal{K}}({\boldsymbol{x}_{\boldsymbol{q}}}^i)\right)(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = \\ &-\boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^i - \dot{\boldsymbol{q}}_n) + \Delta t\ \boldsymbol{F}({\boldsymbol{x}_{\boldsymbol{q}}}^i) + \Delta t\ \boldsymbol{\mathcal{K}}({\boldsymbol{x}_{\boldsymbol{q}}}^i)(-\boldsymbol{q}^i + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^i) \end{aligned} \tag{116}$$

From Equation 318, we can deduce $\boldsymbol{q}^{i+1} - \boldsymbol{q}^i$:

$$
\begin{aligned}
\boldsymbol{q}^{i+1} - \boldsymbol{q}^{i} &= -\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i} - (-\Delta t\ \boldsymbol{I})(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^{i}) \\
&= -\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i} + \Delta t\ (\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^{i}) \\
&= -\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i+1}
\end{aligned} \tag{117}
$$

Then

$$
\boldsymbol{q}^{i+1} = \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i+1} \tag{118}
$$

7.2.2 Solve for $\boldsymbol{q}$

Using the Schur complement (see Equation 321), we obtain the reduced equation in $\boldsymbol{q}^{i+1} - \boldsymbol{q}^{i}$:

$$
\begin{gathered}
\left((-\Delta t\ \boldsymbol{\mathcal{K}}(\boldsymbol{x_q}{}^{i})) - (M - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{x_q}{}^{i}))\left(-\frac{1}{\Delta t} I\right)\right)(\boldsymbol{q}^{i+1} - \boldsymbol{q}^{i}) = \\
-M(\dot{\boldsymbol{q}}^{i} - \dot{\boldsymbol{q}}_n) + \Delta t\ \boldsymbol{F}(\boldsymbol{x_q}{}^{i}) - (M - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{x_q}{}^{i}))\left(-\frac{1}{\Delta t}\right)(-\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i})
\end{gathered} \tag{119}
$$

Cleaning:

$$
\begin{gathered}
\left(\frac{1}{\Delta t} M - \boldsymbol{\mathcal{B}}(\boldsymbol{x_q}{}^{i}) - \Delta t\ \boldsymbol{\mathcal{K}}(\boldsymbol{x_q}{}^{i})\right)(\boldsymbol{q}^{i+1} - \boldsymbol{q}^{i}) = \\
-M(\dot{\boldsymbol{q}}^{i} - \dot{\boldsymbol{q}}_n) + \Delta t\ \boldsymbol{F}(\boldsymbol{x_q}{}^{i}) + \frac{1}{\Delta t}(M - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{x_q}{}^{i}))(-\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i})
\end{gathered} \tag{120}
$$

7.2.3 Rayleigh Damping

F_{Rayleigh} (Equation 32) is added to the sum of forces in Equation 104:

$$
\begin{aligned}
M(\dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n) &= \Delta t\ \left(F(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) + F_{\text{Rayleigh}}\right) \\
&= \Delta t\ (F(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_{n+1})
\end{aligned} \tag{121}
$$

We define the residual function r such that:

$$
r(\boldsymbol{x_q}) = \begin{bmatrix} \boldsymbol{q} - \boldsymbol{q}_n - \Delta t\ \dot{\boldsymbol{q}} \\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}} - \dot{\boldsymbol{q}}_n) - \Delta t\ \left(\boldsymbol{F}(\boldsymbol{x_q}) + (-\alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}})\dot{\boldsymbol{q}}_{n+1}\right) \end{bmatrix} = \begin{bmatrix} r_1(\boldsymbol{x_q}) \\ r_2(\boldsymbol{x_q}) \end{bmatrix} \tag{122}
$$

The nonlinear equation to solve is $r(\boldsymbol{q}, \dot{\boldsymbol{q}}) = 0$

The derivatives of r_1 with respect to $\boldsymbol{q}$ and $\dot{\boldsymbol{q}}$ can be found respectively in Equation 108 and Equation 109.

$$
\frac{\partial r_2}{\partial \boldsymbol{q}} = -\Delta t \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}} = -\Delta t\ \boldsymbol{\mathcal{K}} \tag{123}
$$

$$
\begin{aligned}
\frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} &= \boldsymbol{\mathcal{M}} - \Delta t\left(\frac{\partial \boldsymbol{F}}{\partial \dot{\boldsymbol{q}}} - \alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}}\right) \\
&= (1 + \alpha\Delta t)\boldsymbol{\mathcal{M}} - \Delta t\boldsymbol{\mathcal{B}} - \beta\Delta t\ \boldsymbol{\mathcal{K}}
\end{aligned} \tag{124}
$$

The Jacobian of r:

$$
J_r = \frac{\partial r}{\partial \boldsymbol{x_q}} = \begin{bmatrix} I & -\Delta t I \\ -\Delta t\ \boldsymbol{\mathcal{K}} & (1 + \alpha\Delta t)\boldsymbol{\mathcal{M}} - \Delta t\boldsymbol{\mathcal{B}} - \beta\Delta t\ \boldsymbol{\mathcal{K}} \end{bmatrix} \tag{125}
$$

Newton-Raphson to solve $r(\boldsymbol{x_q}) = 0$:

$$
\begin{gathered}
\begin{bmatrix} I & -\Delta t I \\ -\Delta t\ \boldsymbol{\mathcal{K}} & (1 + \alpha\Delta t)\boldsymbol{\mathcal{M}} - \Delta t\boldsymbol{\mathcal{B}} - \beta\Delta t\ \boldsymbol{\mathcal{K}} \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^{i} \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^{i} \end{bmatrix} = \\
\begin{bmatrix} -\boldsymbol{q}^{i} + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^{i} \\ -\boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^{i} - \dot{\boldsymbol{q}}_n) + \Delta t\ \left(\boldsymbol{F}(\boldsymbol{x_q}{}^{i}) + (-\alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}})\dot{\boldsymbol{q}}_{n+1}\right) \end{bmatrix}
\end{gathered} \tag{126}
$$

Solve for $\dot{\boldsymbol{q}}$

Using the Schur complement (see Equation 319), we obtain the reduced equation in $\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i$:

$$\begin{gathered}(((1+\alpha\Delta t)\boldsymbol{\mathcal{M}} - \Delta t\boldsymbol{\mathcal{B}} - \beta\Delta t\ \boldsymbol{\mathcal{K}}) - (-\Delta t\ \boldsymbol{\mathcal{K}})(-\Delta t))(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = \\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^i - \dot{\boldsymbol{q}}_n) + \Delta t\ \left(\boldsymbol{F}(\boldsymbol{x_q}{}^i) + (-\alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}})\dot{\boldsymbol{q}}_{n+1}\right) - (-\Delta t\ \boldsymbol{\mathcal{K}})(-\boldsymbol{q}^i + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^i)\end{gathered} \tag{127}$$

Cleaning:

$$\begin{gathered}\Big((1+\alpha\Delta t)\boldsymbol{\mathcal{M}} - \Delta t\boldsymbol{\mathcal{B}} - \Delta t(\beta + \Delta t)\ \boldsymbol{\mathcal{K}}\Big)(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = \\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}^i - \dot{\boldsymbol{q}}_n) + \Delta t\ \left(\boldsymbol{F}(\boldsymbol{x_q}{}^i) + (-\alpha\boldsymbol{\mathcal{M}} + \beta\boldsymbol{\mathcal{K}})\dot{\boldsymbol{q}}_{n+1} + \boldsymbol{\mathcal{K}}(-\boldsymbol{q}^i + \boldsymbol{q}_n + \Delta t\ \dot{\boldsymbol{q}}^i)\right)\end{gathered} \tag{128}$$

7.2.4 Force Linearization

Equation 104 is a nonlinear equation. Instead of solving it iteratively, we use an approximation of the expression of forces.

Let's define:

$$\Delta\boldsymbol{q} = \boldsymbol{q}_{n+1} - \boldsymbol{q}_n \tag{129}$$

$$\Delta\dot{\boldsymbol{q}} = \dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n \tag{130}$$

From Equation 104, we can deduce:

$$\Delta\boldsymbol{q} = \Delta t\ \dot{\boldsymbol{q}}_{n+1} = \Delta t(\Delta\dot{\boldsymbol{q}} + \dot{\boldsymbol{q}}_n) \tag{131}$$

$$\Delta\dot{\boldsymbol{q}} = \frac{1}{\Delta t}(\boldsymbol{q}_{n+1} - \boldsymbol{q}_n) - \dot{\boldsymbol{q}}_n = \frac{1}{\Delta t}\Delta\boldsymbol{q} - \dot{\boldsymbol{q}}_n \tag{132}$$

Taylor series expansion of F around $(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)$:

$$\begin{aligned}\boldsymbol{F}(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) &= \boldsymbol{F}(\boldsymbol{q}_n + \Delta\boldsymbol{q}, \dot{\boldsymbol{q}}_n + \Delta\dot{\boldsymbol{q}}) \\ &= \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \frac{\partial\boldsymbol{F}}{\partial\boldsymbol{q}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\boldsymbol{q} + \frac{\partial\boldsymbol{F}}{\partial\dot{\boldsymbol{q}}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\dot{\boldsymbol{q}} + o(\|\Delta\boldsymbol{q}\|^2, \|\Delta\dot{\boldsymbol{q}}\|^2)\end{aligned} \tag{133}$$

$\boldsymbol{F}$ is approximated:

$$\boldsymbol{F}(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) \approx \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \underbrace{\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{q}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)}_{\boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)}\Delta\boldsymbol{q} + \underbrace{\frac{\partial\boldsymbol{F}}{\partial\dot{\boldsymbol{q}}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)}_{\boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)}\Delta\dot{\boldsymbol{q}} \tag{134}$$

Second line of Equation 104 becomes:

$$\boldsymbol{\mathcal{M}}\ \Delta\dot{\boldsymbol{q}} = \Delta t(\boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\boldsymbol{q} + \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\dot{\boldsymbol{q}}) \tag{135}$$

Solving for $\Delta\dot{\boldsymbol{q}}$

Replacing $\Delta\boldsymbol{q}$ from Equation 131 in Equation 135:

$$\boldsymbol{\mathcal{M}}\ \Delta\dot{\boldsymbol{q}} = \Delta t(\boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\ \Delta t\ (\Delta\dot{\boldsymbol{q}} + \dot{\boldsymbol{q}}_n) + \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\dot{\boldsymbol{q}}) \tag{136}$$

Grouping terms in $\Delta\dot{\boldsymbol{q}}$ in LHS:

$$(\boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) - \Delta t^2\ \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n))\Delta\dot{\boldsymbol{q}} = \Delta t\ \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \Delta t^2\boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n \tag{137}$$

Defining $A = \boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) - \Delta t^2\ \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)$ and $b = \Delta t\ \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \Delta t^2\boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\dot{\boldsymbol{q}}_n$, we have a linear system to solve:

$$A\ \Delta\dot{\boldsymbol{q}} = b \tag{138}$$

Then we use Equation 131 to deduce $\Delta\boldsymbol{q}$.

Solving for $\Delta\boldsymbol{q}$

Replacing $\Delta\dot{\boldsymbol{q}}$ from Equation 132 in Equation 135:

$$\boldsymbol{\mathcal{M}}\ \left(\frac{1}{\Delta t}\Delta\boldsymbol{q} - \dot{\boldsymbol{q}}_n\right) = \Delta t\Big(\boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Delta\boldsymbol{q} + \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\Big(\frac{1}{\Delta t}\Delta\boldsymbol{q} - \dot{\boldsymbol{q}}_n\Big)\Big) \tag{139}$$

Grouping terms in $\Delta\boldsymbol{q}$ in LHS:

$$\left(\frac{1}{\Delta t}\boldsymbol{\mathcal{M}} - \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) - \Delta t \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)\right)\Delta \boldsymbol{q} = \Delta t\ \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (\boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n))\dot{\boldsymbol{q}}_n \tag{140}$$

Defining $A = \frac{1}{\Delta t}\boldsymbol{\mathcal{M}} - \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) - \Delta t \boldsymbol{\mathcal{K}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n)$ and $b = \Delta t\ \boldsymbol{F}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (\boldsymbol{\mathcal{M}} - \Delta t\ \boldsymbol{\mathcal{B}}(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n))\dot{\boldsymbol{q}}_n$, we have a linear system to solve:

$$A\ \Delta \boldsymbol{q} = b \tag{141}$$

Then we use Equation 132 to deduce $\Delta\dot{\boldsymbol{q}}$.

7.2.5 Force Linearization with Rayleigh Damping

$$\begin{aligned} F(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) + F_{\text{Rayleigh},n+1} \approx & F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + F_{\text{Rayleigh},n} \\ & + \left(\underbrace{\frac{\partial F}{\partial x}}_{K} + \underbrace{\frac{\partial F_{\text{Rayleigh}}}{\partial x}}_{0}\right)\Delta x \\ & + \left(\underbrace{\frac{\partial F}{\partial v}}_{B} + \underbrace{\frac{\partial F_{\text{Rayleigh}}}{\partial v}}_{-\alpha M + \beta K}\right)\Delta v \end{aligned} \tag{142}$$

$$\begin{aligned} F(\boldsymbol{q}_{n+1}, \dot{\boldsymbol{q}}_{n+1}) + F_{\text{Rayleigh},n+1} \approx & F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_n \\ & + K\ \Delta x + (B - \alpha M + \beta K)\Delta v \end{aligned} \tag{143}$$

Equation 104 becomes:

$$M\ \Delta v = \Delta t (F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_n + K\ \Delta x + (B - \alpha M + \beta K)\Delta v) \tag{144}$$

Solving for Δv

Replacing Δx from Equation 131 in Equation 144:

$$M\ \Delta v = \Delta t (F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_n + K\ \Delta t(\Delta v + \dot{\boldsymbol{q}}_n) + (B - \alpha M + \beta K)\Delta v) \tag{145}$$

Grouping terms in Δv in LHS:

$$\begin{aligned} ((1 + \alpha \Delta t)M - \Delta t B - \Delta t(\Delta t + \beta)K)\Delta v = & \Delta t\ F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) \\ & + \Delta t\ (-\alpha M + (\beta + \Delta t)K)\dot{\boldsymbol{q}}_n \end{aligned} \tag{146}$$

Solving for Δx

Replacing Δv from Equation 132 in Equation 144:

$$\begin{gathered} M\left(\frac{1}{\Delta t}\Delta x - \dot{\boldsymbol{q}}_n\right) = \\ \Delta t\left(F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_n + K\ \Delta x + (B - \alpha M + \beta K)\left(\frac{1}{\Delta t}\Delta x - \dot{\boldsymbol{q}}_n\right)\right) \end{gathered} \tag{147}$$

Grouping terms in Δx in LHS:

$$\begin{gathered} \left(M\left(\frac{1}{\Delta t}\right) - \Delta t\ K - (B - \alpha M + \beta K)\right)\Delta x = \\ \Delta t (F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + (-\alpha M + \beta K)\dot{\boldsymbol{q}}_n - (B - \alpha M + \beta K)\dot{\boldsymbol{q}}_n) + M\dot{\boldsymbol{q}}_n \end{gathered} \tag{148}$$

$$\left(\frac{1}{\Delta t}\left(\frac{1}{\Delta t} + \alpha\right)M - \frac{1}{\Delta t}B - \left(1 + \frac{\beta}{\Delta t}\right)\right)\Delta x = F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \Delta t\ M\dot{\boldsymbol{q}}_n - B\dot{\boldsymbol{q}}_n \tag{149}$$

7.3 Crank–Nicolson method

It is the average of the forward Euler method (Equation 90) and the backward Euler method (Equation 104)

$$\underbrace{\frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1}-\boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1}-\dot{\boldsymbol{q}}_n)\end{bmatrix}}_{\text{forward}}+\underbrace{\frac{1}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1}-\boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1}-\dot{\boldsymbol{q}}_n)\end{bmatrix}}_{\text{backward}}=\underbrace{\begin{bmatrix}\dot{\boldsymbol{q}}_n\\ \boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)\end{bmatrix}}_{\text{forward}}+\underbrace{\begin{bmatrix}\dot{\boldsymbol{q}}_{n+1}\\ \boldsymbol{F}(\boldsymbol{q}_{n+1},\dot{\boldsymbol{q}}_{n+1})\end{bmatrix}}_{\text{backward}} \tag{150}$$

$$\frac{2}{\Delta t}\begin{bmatrix}\boldsymbol{q}_{n+1}-\boldsymbol{q}_n\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}_{n+1}-\dot{\boldsymbol{q}}_n)\end{bmatrix}=\begin{bmatrix}\dot{\boldsymbol{q}}_n+\dot{\boldsymbol{q}}_{n+1}\\ \boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+\boldsymbol{F}(\boldsymbol{q}_{n+1},\dot{\boldsymbol{q}}_{n+1})\end{bmatrix} \tag{151}$$

Definition of the residual function r:

$$r(\boldsymbol{x}_{\boldsymbol{q}})=r(\boldsymbol{q},\dot{\boldsymbol{q}})=\begin{bmatrix}\boldsymbol{q}-\boldsymbol{q}_n-\frac{\Delta t}{2}(\dot{\boldsymbol{q}}_n+\dot{\boldsymbol{q}})\\ \boldsymbol{\mathcal{M}}(\dot{\boldsymbol{q}}-\dot{\boldsymbol{q}}_n)-\frac{\Delta t}{2}(\boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+\boldsymbol{F}(\boldsymbol{q},\dot{\boldsymbol{q}}))\end{bmatrix} \tag{152}$$

Based on Equation 151, we want to find the root $\boldsymbol{x}_{\boldsymbol{q}_{n+1}}=\begin{bmatrix}\boldsymbol{q}_{n+1}\\ \dot{\boldsymbol{q}}_{n+1}\end{bmatrix}$ of r such that $r\left(\boldsymbol{x}_{\boldsymbol{q}_{n+1}}\right)=0$.

We will need to compute the Jacobian $J_r=\frac{\partial r}{\partial x}=\begin{bmatrix}\frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \dot{\boldsymbol{q}}}\\ \frac{\partial r_2}{\partial \boldsymbol{q}} & \frac{\partial r_2}{\partial \dot{\boldsymbol{q}}}\end{bmatrix}$ of r. Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}}=\boldsymbol{I} \tag{153}$$

$$\frac{\partial r_1}{\partial \dot{\boldsymbol{q}}}=-\frac{\Delta t}{2}\ \boldsymbol{I} \tag{154}$$

$$\frac{\partial r_2}{\partial \boldsymbol{q}}=-\frac{\Delta t}{2}\frac{\partial F}{\partial \boldsymbol{q}}=-\frac{\Delta t}{2}\ K \tag{155}$$

$$\frac{\partial r_2}{\partial \dot{\boldsymbol{q}}}=M-\frac{\Delta t}{2}\frac{\partial F}{\partial \dot{\boldsymbol{q}}}=M-\frac{\Delta t}{2}\ B \tag{156}$$

The final expression of the Jacobian is:

$$J_r=\begin{bmatrix}\boldsymbol{I} & -\frac{\Delta t}{2}\ \boldsymbol{I}\\ -\frac{\Delta t}{2}\ K & M-\frac{\Delta t}{2}\ B\end{bmatrix} \tag{157}$$

Newton-Raphson to solve $r(\boldsymbol{x}_{\boldsymbol{q}})=0$:

$$\begin{bmatrix}\boldsymbol{I} & -\frac{\Delta t}{2}\ \boldsymbol{I}\\ -\frac{\Delta t}{2}\ K & \boldsymbol{\mathcal{M}}-\frac{\Delta t}{2}\ B\end{bmatrix}\begin{bmatrix}\boldsymbol{q}^{i+1}-\boldsymbol{q}^i\\ \dot{\boldsymbol{q}}^{i+1}-\dot{\boldsymbol{q}}^i\end{bmatrix}=\begin{bmatrix}-\boldsymbol{q}^i+\boldsymbol{q}_n+\frac{\Delta t}{2}(\dot{\boldsymbol{q}}_n+\dot{\boldsymbol{q}}^i)\\ -M(\dot{\boldsymbol{q}}^i-\dot{\boldsymbol{q}}_n)+\frac{\Delta t}{2}(\boldsymbol{F}(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+\boldsymbol{F}(\boldsymbol{q}^i,\dot{\boldsymbol{q}}^i))\end{bmatrix} \tag{158}$$

7.3.1 Force Linearization

Replacing the linearized force from Equation 134 in the bottom row of Equation 151:

$$M\ \Delta v=\frac{1}{2}\Delta t(2F(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+K\Delta x+B\Delta v) \tag{159}$$

Solve for Δv

Replacing Δx from in Equation 159:

$$M\ \Delta v=\frac{1}{2}\Delta t\left(2F(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+K\frac{1}{2}\ \Delta t(\Delta v+2\dot{\boldsymbol{q}}_n)+B\Delta v\right) \tag{160}$$

Grouping terms in Δv in LHS:

$$\left(M-\frac{1}{2}\Delta t\ B-\frac{1}{4}\Delta t^2\ K\right)\Delta v=\Delta t\ F(\boldsymbol{q}_n,\dot{\boldsymbol{q}}_n)+\frac{1}{2}\Delta t^2 K\dot{\boldsymbol{q}}_n \tag{161}$$

7.3.2 Force Linearization with Rayleigh Damping

Replacing the linearized force from Equation 143 in the bottom row of Equation 151:

$$
\begin{aligned}
M\ \Delta v = \frac{1}{2}\Delta t[2F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + 2(-\alpha M + \beta K)\dot{\boldsymbol{q}}_n \\
+K\ \Delta x + (B - \alpha M + \beta K)\Delta v]
\end{aligned}
\tag{162}
$$

Solve for Δv

Replacing Δx from in Equation 159:

$$
\begin{aligned}
&\left[\left(1 + \frac{1}{2}\alpha\Delta t\right)M - \frac{1}{2}\Delta t B - \frac{1}{2}\Delta t\left(\frac{1}{2}\Delta t + \beta\right)K\right]\Delta v \\
&= \Delta t\ F(\boldsymbol{q}_n, \dot{\boldsymbol{q}}_n) + \Delta t\left(-\alpha M + \left(\beta + \frac{1}{2}\Delta t\right)K\right)\dot{\boldsymbol{q}}_n
\end{aligned}
\tag{163}
$$

7.4 2-step BDF

In Equation 56, the time derivative can be approximated using the backward first-order finite differences:

$$
y'_{n+2} \approx \frac{3y_{n+2} - 4y_{n+1} + y_n}{2\Delta t}
\tag{164}
$$

Equation 56 becomes:

$$
\begin{aligned}
\frac{3y_{n+2} - 4y_{n+1} + y_n}{2\Delta t} &= f(t_{n+2}, y_{n+2}) \\
\Leftrightarrow y_{n+2} - \frac{4}{3}y_{n+1} + \frac{1}{3}y_n &= \frac{2}{3}\Delta t\ f(t_{n+2}, y_{n+2})
\end{aligned}
\tag{165}
$$

We observe that the method enters into the category of linear multistep methods (Equation 58) with:

$$
\begin{cases}
s &= 2 \\
a_2 &= 1 \\
a_1 &= -\frac{4}{3} \\
a_0 &= \frac{1}{3} \\
b_2 &= \frac{2}{3} \\
b_1 &= 0 \\
b_0 &= 0
\end{cases}
\tag{166}
$$

We apply this equation on y from Equation 77 and f from Equation 78:

$$
\begin{bmatrix} \boldsymbol{q}_{n+2} - \frac{4}{3}\boldsymbol{q}_{n+1} + \frac{1}{3}\boldsymbol{q}_n \\ \dot{\boldsymbol{q}}_{n+2} - \frac{4}{3}\dot{\boldsymbol{q}}_{n+1} + \frac{1}{3}\dot{\boldsymbol{q}}_n \end{bmatrix} = \frac{2}{3}\Delta t \begin{bmatrix} \dot{\boldsymbol{q}}_{n+2} \\ \boldsymbol{\mathcal{M}}^{-1}\boldsymbol{F}(\boldsymbol{q}_{n+2}, \dot{\boldsymbol{q}}_{n+2}) \end{bmatrix}
\tag{167}
$$

We multiply the second line by $\boldsymbol{\mathcal{M}}$ to get rid of the inverse:

$$
\begin{bmatrix} \boldsymbol{q}_{n+2} - \frac{4}{3}\boldsymbol{q}_{n+1} + \frac{1}{3}\boldsymbol{q}_n \\ \boldsymbol{\mathcal{M}}\left(\dot{\boldsymbol{q}}_{n+2} - \frac{4}{3}\dot{\boldsymbol{q}}_{n+1} + \frac{1}{3}\dot{\boldsymbol{q}}_n\right) \end{bmatrix} = \frac{2}{3}\Delta t \begin{bmatrix} \dot{\boldsymbol{q}}_{n+2} \\ \boldsymbol{F}(\boldsymbol{q}_{n+2}, \dot{\boldsymbol{q}}_{n+2}) \end{bmatrix}
\tag{168}
$$

Definition of the residual function r:

$$
r(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \begin{bmatrix} \boldsymbol{q} - \frac{4}{3}\boldsymbol{q}_{n+1} + \frac{1}{3}\boldsymbol{q}_n - \frac{2}{3}\Delta t\ \dot{\boldsymbol{q}} \\ \boldsymbol{\mathcal{M}}\left(\dot{\boldsymbol{q}} - \frac{4}{3}\dot{\boldsymbol{q}}_{n+1} + \frac{1}{3}\dot{\boldsymbol{q}}_n\right) - \frac{2}{3}\Delta t\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{bmatrix} = \begin{bmatrix} r_1(\boldsymbol{x}_{\boldsymbol{q}}) \\ r_2(\boldsymbol{x}_{\boldsymbol{q}}) \end{bmatrix}
\tag{169}
$$

Based on Equation 168, we want to find the root $\boldsymbol{x}_{\boldsymbol{q}_{n+1}} = \begin{bmatrix} \boldsymbol{q}_{n+1} \\ \dot{\boldsymbol{q}}_{n+1} \end{bmatrix}$ of r such that $r\left(\boldsymbol{x}_{\boldsymbol{q}_{n+1}}\right) = 0$.

We will need to compute the Jacobian $J_r = \frac{\partial r}{\partial x} = \begin{bmatrix} \frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} \\ \frac{\partial r_2}{\partial \boldsymbol{q}} & \frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} \end{bmatrix}$ of r. Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = \boldsymbol{I} \tag{170}$$

$$\frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} = -\frac{2}{3}\Delta t\ \boldsymbol{I} \tag{171}$$

$$\frac{\partial r_2}{\partial \boldsymbol{q}} = -\frac{2}{3}\Delta t\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}} = -\frac{2}{3}\Delta t\ \boldsymbol{\mathcal{K}} \tag{172}$$

$$\frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} = \boldsymbol{\mathcal{M}} - \frac{2}{3}\Delta t\frac{\partial F}{\partial \dot{\boldsymbol{q}}} = \boldsymbol{\mathcal{M}} - \frac{2}{3}\Delta t\ \boldsymbol{\mathcal{B}} \tag{173}$$

The final expression of the Jacobian is:

$$J_r = \begin{bmatrix} \boldsymbol{I} & -\frac{2}{3}\Delta t\ \boldsymbol{I} \\ -\frac{2}{3}\Delta t\ \boldsymbol{\mathcal{K}} & \boldsymbol{\mathcal{M}} - \frac{2}{3}\Delta t\ \boldsymbol{\mathcal{B}} \end{bmatrix} \tag{174}$$

Newton-Raphson to solve $r(\boldsymbol{x_q}) = 0$:

$$\begin{bmatrix} \boldsymbol{I} & -\frac{2}{3}\Delta t\ \boldsymbol{I} \\ -\frac{2}{3}\Delta t\ \boldsymbol{\mathcal{K}} & \boldsymbol{\mathcal{M}} - \frac{2}{3}\Delta t\ \boldsymbol{\mathcal{B}} \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \end{bmatrix} = \begin{bmatrix} -r_1(\boldsymbol{x_q}^i) \\ -r_2(\boldsymbol{x_q}^i) \end{bmatrix} \tag{175}$$

7.5 Newmark

7.6 Implicit Linear Multistep Methods

Based on Equation 58, let's define the residual function as:

$$r(x) = a_s x + \sum_{j=0}^{s-1} a_j y_{n+j} - \Delta t\left(b_s f(t_{n+s}, x) + \sum_{j=0}^{s-1} b_j f(t_{n+j}, y_{n+j})\right) \tag{176}$$

To find the next unknown state y_{n+s}, we need to compute the root x_r of r such that $r(x_r) = 0$. Newton-Raphson algorithm can be applied.

In the case of the Newton's second law (Equation 31),

$$\begin{aligned} r(\boldsymbol{x_q}) = r(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \\ a_s\begin{bmatrix} \boldsymbol{q} \\ \boldsymbol{\mathcal{M}}\dot{\boldsymbol{q}} \end{bmatrix} + \sum_{j=0}^{s-1} a_j \begin{bmatrix} \boldsymbol{q}_{n+j} \\ \boldsymbol{\mathcal{M}}\dot{\boldsymbol{q}}_{n+j} \end{bmatrix} - \Delta t\left(b_s\begin{bmatrix} \dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{bmatrix} + \sum_{j=0}^{s-1} b_j \begin{bmatrix} \dot{\boldsymbol{q}}_{n+j} \\ \boldsymbol{F}(\boldsymbol{q}_{n+j}, \dot{\boldsymbol{q}}_{n+j}) \end{bmatrix}\right) \\ = \begin{bmatrix} r_1(\boldsymbol{x_q}) \\ r_2(\boldsymbol{x_q}) \end{bmatrix} \end{aligned} \tag{177}$$

We will need to compute the Jacobian $J_r = \frac{\partial r}{\partial x} = \begin{bmatrix} \frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} \\ \frac{\partial r_2}{\partial \boldsymbol{q}} & \frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} \end{bmatrix}$ of r. Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = a_s \boldsymbol{I} \tag{178}$$

$$\frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} = -\Delta t\ b_s\ \boldsymbol{I} \tag{179}$$

$$\frac{\partial r_2}{\partial \boldsymbol{q}} = -\Delta t\ b_s\ \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}} = -\Delta t\ b_s\ \boldsymbol{\mathcal{K}} \tag{180}$$

$$\frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} = a_s\boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \frac{\partial \boldsymbol{F}}{\partial \dot{\boldsymbol{q}}} = a_s\boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}} \tag{181}$$

The final expression of the Jacobian is:

$$J_r = \begin{bmatrix} a_s \boldsymbol{I} & -\Delta t\ b_s\ \boldsymbol{I} \\ -\Delta t\ b_s\ \boldsymbol{\mathcal{K}} & a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}} \end{bmatrix} \tag{182}$$

We define $\boldsymbol{\mathcal{K}}^i = \boldsymbol{\mathcal{K}}(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i)$ and $\boldsymbol{\mathcal{B}}^i = \boldsymbol{\mathcal{B}}(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i)$.

Newton-Raphson to solve $r(\boldsymbol{x}_{\boldsymbol{q}}) = 0$:

$$\begin{bmatrix} a_s \boldsymbol{I} & -\Delta t\ b_s\ \boldsymbol{I} \\ -\Delta t\ b_s\ \boldsymbol{\mathcal{K}}^i & a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}}^i \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \end{bmatrix} = -r(\boldsymbol{x}_{\boldsymbol{q}}{}^i) \tag{183}$$

7.6.1 Solve for $\dot{\boldsymbol{q}}$

Using the Schur complement (see Equation 319), we obtain the reduced equation in $\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i$:

$$\left(a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}}^i - \Delta t^2 \frac{b_s^2}{a_s} \boldsymbol{\mathcal{K}}^i \right) (\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = -r_2(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) - \Delta t \frac{b_s}{a_s} \boldsymbol{\mathcal{K}}^i r_1(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) \tag{184}$$

Equation 184 is a linear system of the form

$$A^i x^i = b^i \tag{185}$$

where

$$\begin{cases} A^i = a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}}^i - \Delta t^2 \frac{b_s^2}{a_s} \boldsymbol{\mathcal{K}}^i \\ x^i = \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ b^i = -r_2(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) - \Delta t \frac{b_s}{a_s} \boldsymbol{\mathcal{K}}^i r_1(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) \end{cases} \tag{186}$$

From Equation 318, we can deduce $\boldsymbol{q}^{i+1} - \boldsymbol{q}^i$:

$$\boldsymbol{q}^{i+1} - \boldsymbol{q}^i = \frac{1}{a_s} \left(-r_1(\boldsymbol{x}_{\boldsymbol{q}}{}^i) + \Delta t\ b_s (\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) \right) \tag{187}$$

7.6.2 Rayleigh Damping

$$\begin{gathered} r(\boldsymbol{x}_{\boldsymbol{q}}) = r(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \\ a_s \begin{bmatrix} \boldsymbol{q} \\ \boldsymbol{\mathcal{M}} \dot{\boldsymbol{q}} \end{bmatrix} + \sum_{j=0}^{s-1} a_j \begin{bmatrix} \boldsymbol{q}_{n+j} \\ \boldsymbol{\mathcal{M}} \dot{\boldsymbol{q}}_{n+j} \end{bmatrix} \\ -\Delta t \left(b_s \begin{bmatrix} \dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + (-\alpha \boldsymbol{\mathcal{M}} + \beta \boldsymbol{\mathcal{K}}(\boldsymbol{q}, \dot{\boldsymbol{q}})) \dot{\boldsymbol{q}} \end{bmatrix} + \right. \\ \left. \sum_{j=0}^{s-1} b_j \begin{bmatrix} \dot{\boldsymbol{q}}_{n+j} \\ \boldsymbol{F}(\boldsymbol{q}_{n+j}, \dot{\boldsymbol{q}}_{n+j}) + (-\alpha \boldsymbol{\mathcal{M}} + \beta \boldsymbol{\mathcal{K}}(\boldsymbol{q}_{n+j}, \dot{\boldsymbol{q}}_{n+j})) \dot{\boldsymbol{q}} \end{bmatrix} \right) \\ = \begin{bmatrix} r_1(\boldsymbol{x}_{\boldsymbol{q}}) \\ r_2(\boldsymbol{x}_{\boldsymbol{q}}) \end{bmatrix} \end{gathered} \tag{188}$$

Only the second line is modified, so only the derivatives of r_2 must be computed:

$$\frac{\partial r_2}{\partial \boldsymbol{q}} = -\Delta t\ b_s \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{q}} = -\Delta t\ b_s\ \boldsymbol{\mathcal{K}} \tag{189}$$

$$\begin{aligned} \frac{\partial r_2}{\partial \dot{\boldsymbol{q}}} &= a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s \left(\frac{\partial \boldsymbol{F}}{\partial \dot{\boldsymbol{q}}} - \alpha \boldsymbol{\mathcal{M}} + \beta \boldsymbol{\mathcal{K}} \right) \\ &= a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ (\boldsymbol{\mathcal{B}} - \alpha \boldsymbol{\mathcal{M}} + \beta \boldsymbol{\mathcal{K}}) \\ &= (a_s + \Delta t\ b_s \alpha) \boldsymbol{\mathcal{M}} - \Delta t\ b_s (\boldsymbol{\mathcal{B}} + \beta \boldsymbol{\mathcal{K}}) \end{aligned} \tag{190}$$

The final expression of the Jacobian is:

$$J_r = \begin{bmatrix} a_s \boldsymbol{I} & -\Delta t \ b_s \ \boldsymbol{I} \\ -\Delta t \ b_s \ \boldsymbol{\mathcal{K}} & (a_s + \Delta t \ b_s \alpha)\boldsymbol{\mathcal{M}} - \Delta t \ b_s(\boldsymbol{\mathcal{B}} + \beta \boldsymbol{\mathcal{K}}) \end{bmatrix} \tag{191}$$

Newton-Raphson to solve $r(\boldsymbol{x_q}) = 0$:

$$\begin{bmatrix} a_s \boldsymbol{I} & -\Delta t \ b_s \ \boldsymbol{I} \\ -\Delta t \ b_s \ \boldsymbol{\mathcal{K}} & (a_s + \Delta t \ b_s \alpha)\boldsymbol{\mathcal{M}} - \Delta t \ b_s(\boldsymbol{\mathcal{B}} + \beta \boldsymbol{\mathcal{K}}) \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \end{bmatrix} = -r(\boldsymbol{x_q}^i) \tag{192}$$

Solve for $\dot{\boldsymbol{q}}$

Using the Schur complement (see Equation 319), we obtain the reduced equation in $\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i$:

$$\begin{gathered} \left((a_s + \Delta t \ b_s \alpha)\boldsymbol{\mathcal{M}} - \Delta t \ b_s \ \boldsymbol{\mathcal{B}}^i - \Delta t \ b_s \left(\beta + \Delta t \frac{b_s}{a_s} \right) \boldsymbol{\mathcal{K}}^i \right) (\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) = \\ -r_2(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) - \Delta t \frac{b_s}{a_s} \boldsymbol{\mathcal{K}}^i r_1(\boldsymbol{q}^i, \dot{\boldsymbol{q}}^i) \end{gathered} \tag{193}$$

From Equation 318, we can deduce $\boldsymbol{q}^{i+1} - \boldsymbol{q}^i$:

$$\boldsymbol{q}^{i+1} - \boldsymbol{q}^i = \frac{1}{a_s} \left(-r_1(\boldsymbol{x_q}^i) + \Delta t \ b_s(\dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i) \right) \tag{194}$$

8 Constraints

8.1 Definitions

Holonomic constraints are relations between position variables:

$$\delta(\boldsymbol{q}, t) = 0 \tag{195}$$

Non-holonomic constraints are relations between velocity variables, or higher time-derivatives of position:

$$\delta(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = 0 \tag{196}$$

Solving both the ODE from Equation 31 and the constraint is a Differential-algebraic system of equations (DAE):

$$\begin{cases} \begin{bmatrix} \frac{d\boldsymbol{q}}{dt} \\ \boldsymbol{\mathcal{M}}\frac{d\dot{\boldsymbol{q}}}{dt} \end{bmatrix} = \begin{bmatrix} \dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) \end{bmatrix} \\ \delta(\boldsymbol{q}, t) \ = 0 \end{cases} \tag{197}$$

8.1.1 Velocity-level equation

We assume that the constraints must be satisfied over time ($\delta(t) = 0$ at all times):

$$\delta = 0 \Leftrightarrow \dot{\delta} = 0 \tag{198}$$

By chain rule:

$$\begin{aligned} \dot{\delta} &= \frac{\partial \delta}{\partial t} \\ &= \frac{\partial \delta}{\partial \boldsymbol{q}} \frac{\partial \boldsymbol{q}}{\partial t} \\ &= \boldsymbol{\mathcal{H}} \dot{\boldsymbol{q}} \end{aligned} \tag{199}$$

This gives an alternative equation to the position-level constraint equation (Equation 195).

8.1.2 Acceleration-level Equation

$$\delta = 0 \Leftrightarrow \dot{\delta} = 0 \Leftrightarrow \ddot{\delta} = 0 \tag{200}$$

By chain rule:

$$\ddot{\delta} = \frac{\partial \dot{\delta}}{\partial t} = \frac{\partial [\boldsymbol{\mathcal{H}} \dot{\boldsymbol{q}}]}{\partial t} = \dot{\boldsymbol{\mathcal{H}}} \dot{\boldsymbol{q}} + \boldsymbol{\mathcal{H}} \ddot{\boldsymbol{q}} \tag{201}$$

$\dot{\boldsymbol{\mathcal{H}}}$ can also be written:

$$\dot{\boldsymbol{\mathcal{H}}} = \frac{\partial \dot{\delta}}{\partial \boldsymbol{q}} \tag{202}$$

8.1.3 Linear Combination

Let's define

$$c(\boldsymbol{x}_{\boldsymbol{q}}, t) = \alpha_{\ddot{\boldsymbol{q}}} \ddot{\delta}(\boldsymbol{x}_{\boldsymbol{q}}, t) + \alpha_{\dot{\boldsymbol{q}}} \dot{\delta}(\boldsymbol{x}_{\boldsymbol{q}}, t) + \alpha_{\boldsymbol{q}} \delta(\boldsymbol{x}_{\boldsymbol{q}}, t) \tag{203}$$

with $\alpha_{\ddot{\boldsymbol{q}}}$, $\alpha_{\dot{\boldsymbol{q}}}$ and $\alpha_{\boldsymbol{q}}$ constant factors.

Constraint equation:

$$c = 0 \tag{204}$$

$$\begin{cases} \alpha_{\ddot{\boldsymbol{q}}} = 0, \alpha_{\dot{\boldsymbol{q}}} = 0, \alpha_{\boldsymbol{q}} = 1 \Rightarrow \text{position-level constraint equation} \\ \alpha_{\ddot{\boldsymbol{q}}} = 0, \alpha_{\dot{\boldsymbol{q}}} = 1, \alpha_{\boldsymbol{q}} = 0 \Rightarrow \text{velocity constraint equation} \\ \alpha_{\ddot{\boldsymbol{q}}} = 1, \alpha_{\dot{\boldsymbol{q}}} = 0, \alpha_{\boldsymbol{q}} = 0 \Rightarrow \text{acceleration-level constraint equation} \end{cases} \tag{205}$$

8.2 Lagrangian

We want to apply C holonomic constraints δ_i, for $0 < i < C-1$. We introduce a Lagrange multiplier λ_i for each of the constraint.

The Lagrangian (Equation 9) is modified by incorporating Lagrange multipliers λ on the holonomic constraints equation:

$$\mathcal{L}'(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) + \sum_{i=0}^{C-1} \lambda_i(t)\delta_i(\boldsymbol{q}, t) \tag{206}$$

Definition:

$$\lambda(t) = \begin{bmatrix} \lambda_0(t) \\ \vdots \\ \lambda_{C-1}(t) \end{bmatrix} \tag{207}$$

$$\delta(t) = \begin{bmatrix} \delta_0(\boldsymbol{q}, t) \\ \vdots \\ \delta_{C-1}(\boldsymbol{q}, t) \end{bmatrix} \tag{208}$$

Using the dot product $\lambda \cdot \delta(\boldsymbol{q}, t) = \sum_{i=0}^{C-1} \lambda_i \delta_i(\boldsymbol{q}, t)$:

$$\mathcal{L}'(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) = \mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}, t) + \lambda \cdot \delta(\boldsymbol{q}, t) \tag{209}$$

We can apply the Euler-Lagrange equation (Equation 21) on the modified Lagrangian:

$$\begin{aligned} &\frac{\partial \mathcal{L}'}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}'}{\partial \dot{\boldsymbol{q}}}\right) = 0 \\ \Rightarrow &\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}}\right) + \left(\frac{\partial \delta}{\partial \boldsymbol{q}}\right)^T \lambda = 0 \end{aligned} \tag{210}$$

This is the Lagrange's equation of the first kind.

We introduce the Jacobian matrix of the constraints $\boldsymbol{\mathcal{H}}$ such that:

$$\boldsymbol{\mathcal{H}}(\boldsymbol{q}, t) = \frac{\partial \delta(\boldsymbol{q}, t)}{\partial \boldsymbol{q}} \tag{211}$$

With n degrees of freedom and m constraints, $\boldsymbol{\mathcal{H}} \in \mathbb{R}^{m \times n}$:

$$\boldsymbol{\mathcal{H}}(\boldsymbol{q}, t) = \begin{bmatrix} \frac{\partial \delta_0}{\partial \boldsymbol{q}_0} & \cdots & \frac{\partial \delta_0}{\partial \boldsymbol{q}_{n-1}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \delta_{m-1}}{\partial \boldsymbol{q}_0} & \cdots & \frac{\partial \delta_{m-1}}{\partial \boldsymbol{q}_{n-1}} \end{bmatrix} \tag{212}$$

8.3 Static

In statics

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{q}} = \boldsymbol{F}(\boldsymbol{q}) \tag{213}$$

and

$$\frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{q}}} = 0 \tag{214}$$

Equation 210 becomes:

$$\begin{cases} \boldsymbol{F}(\boldsymbol{q}) + \boldsymbol{\mathcal{H}}^T \lambda = 0 \\ \delta(\boldsymbol{q}) = 0 \end{cases} \tag{215}$$

This is a nonlinear set of equations of unknowns $(\boldsymbol{q}, \lambda)$ that can be solved using a Newton-Raphson algorithm.

Let's define the residual function r such that:

$$r(\boldsymbol{q}, \lambda) = \begin{bmatrix} \boldsymbol{F}(\boldsymbol{q}) + \boldsymbol{\mathcal{H}}^T \lambda \\ \delta(\boldsymbol{q}) \end{bmatrix} = \begin{bmatrix} r_1(\boldsymbol{q}, \lambda) \\ r_2(\boldsymbol{q}, \lambda) \end{bmatrix} \tag{216}$$

We want to find the root $\boldsymbol{q}_{\text{eq}}, \lambda_{\text{eq}}$ of r such that $r(\boldsymbol{q}_{\text{eq}}, \lambda_{\text{eq}}) = 0$.

We will need to compute the Jacobian J_r of r:

$$J_r = \begin{bmatrix} \frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \lambda} \\ \frac{\partial r_2}{\partial \boldsymbol{q}} & \frac{\partial r_2}{\partial \lambda} \end{bmatrix} \tag{217}$$

Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = \boldsymbol{\mathcal{K}} + \frac{\partial [\boldsymbol{\mathcal{H}}^T \lambda]}{\partial \boldsymbol{q}} \tag{218}$$

We introduce the geometric stiffness $\widetilde{\boldsymbol{\mathcal{K}}}_\lambda$ such as:

$$\widetilde{\boldsymbol{\mathcal{K}}}_{\lambda(\boldsymbol{q}, \lambda)} = \frac{\partial [\boldsymbol{\mathcal{H}}^T \lambda]}{\partial \boldsymbol{q}} \tag{219}$$

Then,

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = \boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda \tag{220}$$

$$\frac{\partial r_1}{\partial \lambda} = \boldsymbol{\mathcal{H}}^T \tag{221}$$

$$\frac{\partial r_2}{\partial \boldsymbol{q}} = \boldsymbol{\mathcal{H}} \tag{222}$$

$$\frac{\partial r_2}{\partial \lambda} = 0 \tag{223}$$

The final expression of the Jacobian J_r is:

$$J_r = \begin{bmatrix} \boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda & \boldsymbol{\mathcal{H}}(\boldsymbol{q})^T \\ \boldsymbol{\mathcal{H}}(\boldsymbol{q}) & 0 \end{bmatrix} \tag{224}$$

Newton-Raphson iteration:

$$J_r \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = -r(\boldsymbol{q}^i, \lambda^i) \tag{225}$$

or,

$$\begin{bmatrix} \boldsymbol{\mathcal{K}}(\boldsymbol{q}^i) + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda(\boldsymbol{q}^i, \lambda^i) & \boldsymbol{\mathcal{H}}(\boldsymbol{q}^i)^T \\ \boldsymbol{\mathcal{H}}(\boldsymbol{q}^i) & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = - \begin{bmatrix} \boldsymbol{F}(\boldsymbol{q}^i) + \boldsymbol{\mathcal{H}}(\boldsymbol{q}^i)^T \lambda^i \\ \delta(\boldsymbol{q}^i) \end{bmatrix} \tag{226}$$

8.3.1 2-steps Solver

We denote $\boldsymbol{\mathcal{H}}^i = \boldsymbol{\mathcal{H}}(\boldsymbol{q}^i)$

Using the Schur complement (Equation 319) on the previous equation, we obtain the reduced equation in $\lambda^{i+1} - \lambda^i$:

$$
\begin{aligned}
&\underbrace{-\mathcal{H}^i\Big(\mathcal{K}(\boldsymbol{q}^i) + \widetilde{\mathcal{K}}_{\lambda(\boldsymbol{q}^i,\lambda^i)}\Big)^{-1}\mathcal{H}^{i^T}}_{\mathcal{W}}(\lambda^{i+1} - \lambda^i) \\
&= -\delta(\boldsymbol{q}^i) + \mathcal{H}^i\Big(\mathcal{K}(\boldsymbol{q}^i) + \widetilde{\mathcal{K}}_{\lambda(\boldsymbol{q}^i)}\Big)^{-1}\Big(\boldsymbol{F}(\boldsymbol{q}^i) + \mathcal{H}^{i^T}\lambda^i\Big)
\end{aligned}
\tag{227}
$$

$\mathcal{W} = \mathcal{H}^i\Big(\mathcal{K}(\boldsymbol{q}^i) + \widetilde{\mathcal{K}}_{\lambda(\boldsymbol{q}^i,\lambda^i)}\Big)^{-1}\mathcal{H}^{i^T}$ is called the compliance matrix.

From Equation 318, we can deduce:

$$
\boldsymbol{q}^{i+1} - \boldsymbol{q}^i = \Big(\mathcal{K}(\boldsymbol{q}^i) + \widetilde{\mathcal{K}}_{\lambda(\boldsymbol{q}^i)}\Big)^{-1}\Big(-\boldsymbol{F}(\boldsymbol{q}^i) - \mathcal{H}^{i^T}\lambda^i\Big) - \mathcal{H}^{i^T}(\lambda^{i+1} - \lambda^i) \tag{228}
$$

8.4 Equation of Motion

Constraint Newton's second law of motion can be deduced from Equation 210 (see also Section 2.1):

$$
\boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) - \mathcal{M}\frac{d\dot{\boldsymbol{q}}}{dt} + \mathcal{H}\big(\boldsymbol{x}_{\boldsymbol{q}}\big)^T\lambda = 0 \tag{229}
$$

By rearranging the terms:

$$
\mathcal{M}\frac{d\dot{\boldsymbol{q}}}{dt} = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + \mathcal{H}\big(\boldsymbol{x}_{\boldsymbol{q}}\big)^T\lambda \tag{230}
$$

8.4.1 Position-level Equation of Motion

$$
\begin{cases}
\frac{d\boldsymbol{q}}{dt} = \dot{\boldsymbol{q}} \\
\mathcal{M}\frac{d\dot{\boldsymbol{q}}}{dt} = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + \mathcal{H}\big(\boldsymbol{x}_{\boldsymbol{q}}\big)^T\lambda \\
\delta(\boldsymbol{q}, t) = 0
\end{cases}
\tag{231}
$$

8.4.2 Velocity-level Equation of Motion

$$
\begin{cases}
\frac{d\boldsymbol{q}}{dt} = \dot{\boldsymbol{q}} \\
\mathcal{M}\frac{d\dot{\boldsymbol{q}}}{dt} = \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + \mathcal{H}\big(\boldsymbol{x}_{\boldsymbol{q}}\big)^T\lambda \\
\mathcal{H}\dot{\boldsymbol{q}} = 0
\end{cases}
\tag{232}
$$

8.5 Linear Multistep Methods

Based on Equation 230, we add the constraint term in the residual function of the linear multistep methods (Section 7.6):

$$
\begin{gathered}
\tilde{r}\big(\boldsymbol{x}_{\boldsymbol{q}}, \lambda\big) = \tilde{r}(\boldsymbol{q}, \dot{\boldsymbol{q}}, \lambda) = \\
a_s\begin{bmatrix}\boldsymbol{q} \\ \mathcal{M}\dot{\boldsymbol{q}}\end{bmatrix} + \sum_{j=0}^{s-1} a_j\begin{bmatrix}\boldsymbol{q}_{n+j} \\ \mathcal{M}\dot{\boldsymbol{q}}_{n+j}\end{bmatrix} \\
-\Delta t\left(b_s\begin{bmatrix}\dot{\boldsymbol{q}} \\ \boldsymbol{F}(\boldsymbol{q}, \dot{\boldsymbol{q}}) + \mathcal{H}(\boldsymbol{q}, t)^T\ \lambda\end{bmatrix} + \sum_{j=0}^{s-1} b_j\begin{bmatrix}\dot{\boldsymbol{q}}_{n+j} \\ \boldsymbol{F}\big(\boldsymbol{q}_{n+j}, \dot{\boldsymbol{q}}_{n+j}\big) + \mathcal{H}\big(\boldsymbol{q}_{n+j}, t_{n+j}\big)^T\ \lambda_{n+j}\end{bmatrix}\right) \\
= \begin{bmatrix}r_1\big(\boldsymbol{x}_{\boldsymbol{q}}, \lambda\big) \\ \tilde{r_2}\big(\boldsymbol{x}_{\boldsymbol{q}}, \lambda\big)\end{bmatrix}
\end{gathered}
\tag{233}
$$

$\tilde{r_2}$ can be related to r_2 from Section 7.6:

$$
\tilde{r_2} = r_2\big(\boldsymbol{x}_{\boldsymbol{q}}\big) - \Delta t\left(b_s\mathcal{H}(\boldsymbol{q}, t)^T\lambda + \sum_{j=0}^{s-1} b_j\mathcal{H}\big(\boldsymbol{q}_{n+j}, t_{n+j}\big)^T\lambda_{n+j}\right) \tag{234}
$$

We know have more unknowns ($\boldsymbol{q}$, $\dot{\boldsymbol{q}}$, λ) than equations, so we add the constraint Equation 195 to $\tilde{r}$:

$$\tilde{r} = \begin{bmatrix} r_1(\boldsymbol{x_q}) \\ \tilde{r_2}(\boldsymbol{x_q}) \\ \delta(\boldsymbol{x_q}, t) \end{bmatrix} \tag{235}$$

We need to compute the Jacobian $J_{\tilde{r}}$ of $\tilde{r}$:

$$J_{\tilde{r}} = \begin{bmatrix} \frac{\partial r_1}{\partial \boldsymbol{q}} & \frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} & \frac{\partial r_1}{\partial \lambda} \\ \frac{\partial \tilde{r_2}}{\partial \boldsymbol{q}} & \frac{\partial \tilde{r_2}}{\partial \dot{\boldsymbol{q}}} & \frac{\partial \tilde{r_2}}{\partial \lambda} \\ \frac{\partial \delta}{\partial \boldsymbol{q}} & \frac{\partial \delta}{\partial \dot{\boldsymbol{q}}} & \frac{\partial \delta}{\partial \lambda} \end{bmatrix} \tag{236}$$

Let's compute each term:

$$\frac{\partial r_1}{\partial \boldsymbol{q}} = a_s \boldsymbol{I} \tag{237}$$

$$\frac{\partial r_1}{\partial \dot{\boldsymbol{q}}} = -\Delta t \; b_s \; \boldsymbol{I} \tag{238}$$

$$\frac{\partial r_1}{\partial \lambda} = 0 \tag{239}$$

$$\frac{\partial \tilde{r_2}}{\partial \boldsymbol{q}} = -\Delta t \; b_s \left(\boldsymbol{\mathcal{K}} + \frac{\partial [\boldsymbol{\mathcal{H}}^T \lambda]}{\partial \boldsymbol{q}} \right) = -\Delta t \; b_s \big(\boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda \big) \tag{240}$$

$$\frac{\partial \tilde{r_2}}{\partial \dot{\boldsymbol{q}}} = a_s \boldsymbol{\mathcal{M}} - \Delta t \; b_s \; \boldsymbol{\mathcal{B}} \tag{241}$$

$$\frac{\partial \tilde{r_2}}{\partial \lambda} = -\Delta t \; b_s \boldsymbol{\mathcal{H}}(\boldsymbol{q})^T \tag{242}$$

$$\frac{\partial \delta}{\partial \boldsymbol{q}} = \boldsymbol{\mathcal{H}}(\boldsymbol{q}) \tag{243}$$

$$\frac{\partial \delta}{\partial \dot{\boldsymbol{q}}} = 0 \tag{244}$$

$$\frac{\partial c}{\partial \lambda} = 0 \tag{245}$$

The final expression of the Jacobian $J_{\tilde{r}}$ is:

$$J_{\tilde{r}} = \begin{bmatrix} a_s \boldsymbol{I} & -\Delta t \; b_s \; \boldsymbol{I} & 0 \\ -\Delta t \; b_s \big(\boldsymbol{\mathcal{K}}(\boldsymbol{x_q}) + \widetilde{\boldsymbol{\mathcal{K}}}_{\lambda(\boldsymbol{q}, \lambda)} \big) & a_s \boldsymbol{\mathcal{M}} - \Delta t \; b_s \; \boldsymbol{\mathcal{B}}(\boldsymbol{x_q}) & -\Delta t \; b_s \boldsymbol{\mathcal{H}}(\boldsymbol{q})^T \\ \boldsymbol{\mathcal{H}}(\boldsymbol{q}) & 0 & 0 \end{bmatrix} \tag{246}$$

We denote $\boldsymbol{\mathcal{H}}^i = \boldsymbol{\mathcal{H}}(\boldsymbol{q}^i)$.

Newton-Raphson to solve $\tilde{r}(\boldsymbol{x_q}) = 0$:

$$\begin{bmatrix} a_s \boldsymbol{I} & -\Delta t \; b_s \; \boldsymbol{I} & 0 \\ -\Delta t \; b_s \big(\boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda \big) & a_s \boldsymbol{\mathcal{M}} - \Delta t \; b_s \; \boldsymbol{\mathcal{B}} & -\Delta t \; b_s {\boldsymbol{\mathcal{H}}^i}^T \\ \boldsymbol{\mathcal{H}}^i & 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{q}^{i+1} - \boldsymbol{q}^i \\ \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = -\tilde{r}(\boldsymbol{x_q}{}^i) \tag{247}$$

We define a block division of the matrix such as:

$$\left[\begin{array}{c|cc} A & B & 0 \\ \hline D & E & F \\ G & 0 & 0 \end{array}\right] = \left[\begin{array}{c|cc} a_s \boldsymbol{I} & -\Delta t\ b_s\ \boldsymbol{I} & 0 \\ \hline -\Delta t\ b_s \left(\boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda\right) & a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}} & -\Delta t\ b_s \boldsymbol{\mathcal{H}}^{i^T} \\ \boldsymbol{\mathcal{H}}^i & 0 & 0 \end{array}\right] \tag{248}$$

Using the Schur complement (Equation 319), we obtain the reduced equation in $\Delta\dot{\boldsymbol{q}}$ and $\Delta\lambda$:

$$\left(\begin{bmatrix} E & F \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} D \\ G \end{bmatrix} A^{-1} [B\ \ 0]\right) \begin{bmatrix} \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = - \begin{bmatrix} \tilde{r_2}\left(\boldsymbol{x_q}^i\right) \\ \tilde{r_3}\left(\boldsymbol{x_q}^i\right) \end{bmatrix} + \begin{bmatrix} D \\ G \end{bmatrix} A^{-1} r_1 \tag{249}$$

$$\Leftrightarrow \begin{bmatrix} E - \frac{1}{a_s} DB & F \\ -\frac{1}{a_s} GB & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = - \begin{bmatrix} \tilde{r_2}\left(\boldsymbol{x_q}^i\right) \\ \tilde{r_3}\left(\boldsymbol{x_q}^i\right) \end{bmatrix} + \frac{1}{a_s} \begin{bmatrix} D \\ G \end{bmatrix} r_1\left(\boldsymbol{x_q}^i\right) \tag{250}$$

Finally:

$$\begin{aligned} &\left[\begin{array}{c|c} a_s \boldsymbol{\mathcal{M}} - \Delta t\ b_s\ \boldsymbol{\mathcal{B}} - \Delta t^2 \frac{b_s^2}{a_s} \left(\boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda\right) & -\Delta t\ b_s \boldsymbol{\mathcal{H}}^{i^T} \\ \hline \Delta t\ \frac{b_s}{a_s} \boldsymbol{\mathcal{H}}^i & 0 \end{array}\right] \begin{bmatrix} \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} \\ &= - \begin{bmatrix} \tilde{r_2} \\ \delta\left(\boldsymbol{x_q}^i\right) \end{bmatrix} + \frac{1}{a_s} \begin{bmatrix} -\Delta t\ b_s \left(\boldsymbol{\mathcal{K}} + \widetilde{\boldsymbol{\mathcal{K}}}_\lambda\right) \\ \boldsymbol{\mathcal{H}}^i \end{bmatrix} r_1\left(\boldsymbol{x_q}^i\right) \end{aligned} \tag{251}$$

We use the notations from Equation 186 and define $A^i_\lambda = A^i - \Delta t^2 \frac{b_s^2}{a_s} \widetilde{\boldsymbol{\mathcal{K}}}_\lambda$ and

$$b^i_\lambda = b^i + \Delta t \left(b_s \boldsymbol{\mathcal{H}}(\boldsymbol{q}, t)^T \lambda + \sum_{j=0}^{s-1} b_j \boldsymbol{\mathcal{H}}\left(\boldsymbol{q}_{n+j}, t_{n+j}\right)^T \lambda_{n+j} \right) - \Delta t \frac{b_s}{a_s} \widetilde{\boldsymbol{\mathcal{K}}}_\lambda r_1\left(\boldsymbol{x_q}^i\right) \tag{252}$$

It yields:

$$\begin{bmatrix} A^i_\lambda & -\Delta t\ b_s \boldsymbol{\mathcal{H}}^{i^T} \\ \Delta t\ \frac{b_s}{a_s} \boldsymbol{\mathcal{H}}^i & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i \\ \lambda^{i+1} - \lambda^i \end{bmatrix} = \begin{bmatrix} b^i_\lambda \\ \delta\left(\boldsymbol{x_q}^i\right) + \frac{1}{a_s} \boldsymbol{\mathcal{H}}^i r_1\left(\boldsymbol{x_q}^i\right) \end{bmatrix} \tag{253}$$

This linear system can be solved directly, or in 2 steps:

2-steps Solver

Using the Schur complement (Equation 319), we obtain the reduced equation in $\lambda^{i+1} - \lambda^i$:

$$\frac{b_s^2}{a_s} \Delta t^2 \boldsymbol{\mathcal{H}}^i A^{i^{-1}}_\lambda \boldsymbol{\mathcal{H}}^{i^T} (\lambda^{i+1} - \lambda^i) = -\delta^i - \frac{1}{a_s} \boldsymbol{\mathcal{H}}^i r_1\left(\boldsymbol{x_q}^i\right) - \Delta t\ \frac{b_s}{a_s} \boldsymbol{\mathcal{H}}^i A^{i^{-1}}_\lambda b^i_\lambda \tag{254}$$

The right-hand side is called constraint violation.

From Equation 318, we can deduce:

$$\begin{aligned} \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i &= A^{i^{-1}}_\lambda \left(b^i_\lambda + \Delta t\ b_s \boldsymbol{\mathcal{H}}^{i^T} (\lambda^{i+1} - \lambda^i)\right) \\ \Leftrightarrow \dot{\boldsymbol{q}}^{i+1} - \dot{\boldsymbol{q}}^i &= \underbrace{A^{i^{-1}}_\lambda b^i_\lambda}_{\text{free motion}} + \underbrace{A^{i^{-1}}_\lambda \Delta t\ b_s \boldsymbol{\mathcal{H}}^{i^T} (\lambda^{i+1} - \lambda^i)}_{\text{corrective motion}} \end{aligned} \tag{255}$$

We define the free motion as:

$$\Delta\dot{\boldsymbol{q}}_{\text{free}}\left(\boldsymbol{x_q}^i, \lambda^i\right) = A^{i^{-1}}_\lambda b^i_\lambda \tag{256}$$

It can be computed independently of the unknowns λ^{i+1}.

The free motion allows to define a free unconstrained velocity $\dot{\boldsymbol{q}}^i_{\text{free}} = \dot{\boldsymbol{q}}^i + \Delta\dot{\boldsymbol{q}}_{\text{free}}$

$\boldsymbol{\mathcal{W}}^i = \boldsymbol{\mathcal{H}}^i A^{i^{-1}}_\lambda \boldsymbol{\mathcal{H}}^{i^T}$ is the compliance matrix projected in the constraint space.

Assuming a single Newton step, $\boldsymbol{x_q}^0 = \boldsymbol{x}_{\boldsymbol{q}_n}$, $\lambda^0 = 0$, and with a backward Euler:

$$\begin{cases} \Delta t^2 \boldsymbol{\mathcal{H}}_n A_\lambda^{-1} \boldsymbol{\mathcal{H}}_n \lambda = -\delta(\boldsymbol{q}_n) - \boldsymbol{\mathcal{H}}_n \Delta t \dot{\boldsymbol{q}}_n - \Delta t \boldsymbol{\mathcal{H}} \Delta \dot{\boldsymbol{q}}_{\text{free}} \\ \dot{\boldsymbol{q}}_{n+1} - \dot{\boldsymbol{q}}_n = A_\lambda^{-1} \left(b + \Delta t^2 \widetilde{\boldsymbol{\mathcal{K}}}_\lambda \dot{\boldsymbol{q}}_n + \Delta t \boldsymbol{\mathcal{H}}^T \lambda \right) \end{cases} \tag{257}$$

8.6 Constraint Linearization

From Equation 137 and Equation 195:

$$\begin{cases} A\ \Delta \dot{\boldsymbol{q}} = b + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \lambda \\ \delta(\boldsymbol{q}_{n+1}) = 0 \end{cases} \tag{258}$$

Taylor series expansion of δ around $\boldsymbol{q}_n$:

$$\delta(\boldsymbol{q}_{n+1}) = \delta(\boldsymbol{q}_n + \Delta \boldsymbol{q}) = \delta(\boldsymbol{q}_n) + \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta \boldsymbol{q} + o(\|\Delta \boldsymbol{q}\|^2) \tag{259}$$

δ is approximated:

$$\delta(\boldsymbol{q}_n + \Delta \boldsymbol{q}) \approx \delta(\boldsymbol{q}_n) + \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta \boldsymbol{q} \tag{260}$$

Replacing $\Delta \boldsymbol{q}$ by Equation 131:

$$\begin{aligned} \delta(\boldsymbol{q}_n + \Delta \boldsymbol{q}) &\approx \delta(\boldsymbol{q}_n) + \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta t (\Delta \dot{\boldsymbol{q}} + \dot{\boldsymbol{q}}_n) \\ &\approx \delta(\boldsymbol{q}_n) + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta \dot{\boldsymbol{q}} + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n \end{aligned} \tag{261}$$

Then,

$$\begin{cases} A\ \Delta \dot{\boldsymbol{q}} = b + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \lambda \\ \delta(\boldsymbol{q}_n) + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta \dot{\boldsymbol{q}} + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n = 0 \end{cases} \tag{262}$$

In matrix format:

$$\begin{bmatrix} A & -\Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \\ \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) & 0 \end{bmatrix} \begin{bmatrix} \Delta \dot{\boldsymbol{q}} \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n \end{bmatrix} \tag{263}$$

Using the Schur complement (Equation 319):

$$\begin{aligned} \Delta t^2 \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) A^{-1} \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \lambda &= -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) A^{-1} b \\ &= -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)(\dot{\boldsymbol{q}}_n + \Delta \dot{\boldsymbol{q}}_{\text{free}}) \\ &\approx -\delta(\boldsymbol{q}_n + \Delta \boldsymbol{q}_{\text{free}}) = -\delta(\boldsymbol{q}_{\text{free}}) \end{aligned} \tag{264}$$

Then,

$$\Delta \dot{\boldsymbol{q}} = A^{-1} \left(b + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \lambda \right) \tag{265}$$

Force and constraint linearization method is equivalent to a single Newton step, ${\boldsymbol{x}_{\boldsymbol{q}}}^0 = \boldsymbol{x}_{\boldsymbol{q}_n}$, $\lambda^0 = 0$, and with a backward Euler.

8.6.1 Multiple Interacting Objects

If the matrix A is made of multiple blocs:

$$A = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \tag{266}$$

We can also divide A^{-1}:

$$A = \begin{bmatrix} A_{00}^{-1} & A_{01}^{-1} \\ A_{10}^{-1} & A_{11}^{-1} \end{bmatrix} \tag{267}$$

The Jacobian matric can also be divided:

$$\boldsymbol{\mathcal{H}} = [\boldsymbol{\mathcal{H}}_0\ \ \boldsymbol{\mathcal{H}}_1] = [\boldsymbol{\mathcal{H}}_0\ \ 0] + [0\ \ \boldsymbol{\mathcal{H}}_1] \tag{268}$$

And the compliance matrix projected into the constraint space:

$$\boldsymbol{\mathcal{W}} = \boldsymbol{\mathcal{H}} A^{-1} \boldsymbol{\mathcal{H}}^T = ([\boldsymbol{\mathcal{H}}_0 \;\; 0] + [0 \;\; \boldsymbol{\mathcal{H}}_1]) A^{-1} \left(\begin{bmatrix} \boldsymbol{\mathcal{H}}_0^T \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \boldsymbol{\mathcal{H}}_1^T \end{bmatrix} \right)$$
$$= [\boldsymbol{\mathcal{H}}_0 \;\; 0] A^{-1} \begin{bmatrix} \boldsymbol{\mathcal{H}}_0^T \\ 0 \end{bmatrix} + [0 \;\; \boldsymbol{\mathcal{H}}_1] A^{-1} \begin{bmatrix} \boldsymbol{\mathcal{H}}_0^T \\ 0 \end{bmatrix} + \tag{269}$$
$$[\boldsymbol{\mathcal{H}}_0 \;\; 0] A^{-1} \begin{bmatrix} 0 \\ \boldsymbol{\mathcal{H}}_1^T \end{bmatrix} + [0 \;\; \boldsymbol{\mathcal{H}}_1] A^{-1} \begin{bmatrix} 0 \\ \boldsymbol{\mathcal{H}}_1^T \end{bmatrix}$$

Let's compute each term:

$$\underbrace{[\boldsymbol{\mathcal{H}}_0 \;\; 0]}_{\in \mathbb{R}^{m \times n}} \underbrace{\underbrace{A^{-1}}_{\in \mathbb{R}^{n \times n}} \underbrace{\begin{bmatrix} \boldsymbol{\mathcal{H}}_0^T \\ 0 \end{bmatrix}}_{\in \mathbb{R}^{n \times m}}}_{\in \mathbb{R}^{n \times m}} = [\boldsymbol{\mathcal{H}}_0 \;\; 0] \begin{bmatrix} A_{00}^{-1} \boldsymbol{\mathcal{H}}_0^T \\ A_{10}^{-1} \boldsymbol{\mathcal{H}}_0^T \end{bmatrix} = \boldsymbol{\mathcal{H}}_0 A_{00}^{-1} \boldsymbol{\mathcal{H}}_0^T \tag{270}$$

Similarly

$$[0 \;\; \boldsymbol{\mathcal{H}}_1] A^{-1} \begin{bmatrix} \boldsymbol{\mathcal{H}}_0^T \\ 0 \end{bmatrix} = [0 \;\; \boldsymbol{\mathcal{H}}_1] \begin{bmatrix} A_{00}^{-1} \boldsymbol{\mathcal{H}}_0^T \\ A_{10}^{-1} \boldsymbol{\mathcal{H}}_0^T \end{bmatrix} = \boldsymbol{\mathcal{H}}_1 A_{10}^{-1} \boldsymbol{\mathcal{H}}_0^T \tag{271}$$

All together:

$$\boldsymbol{\mathcal{H}} A^{-1} \boldsymbol{\mathcal{H}}^T = \boldsymbol{\mathcal{H}}_0 A_{00}^{-1} \boldsymbol{\mathcal{H}}_0^T + \boldsymbol{\mathcal{H}}_1 A_{10}^{-1} \boldsymbol{\mathcal{H}}_0^T + \boldsymbol{\mathcal{H}}_0 A_{01}^{-1} \boldsymbol{\mathcal{H}}_1^T + \boldsymbol{\mathcal{H}}_1 A_{11}^{-1} \boldsymbol{\mathcal{H}}_1^T \tag{272}$$

8.6.2 Relaxation

$\boldsymbol{\mathcal{C}} \lambda = -\delta$

Equation 262 becomes:

$$\begin{cases} A \; \Delta \dot{\boldsymbol{q}} = b + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \lambda \\ \delta(\boldsymbol{q}_n) + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \Delta \dot{\boldsymbol{q}} + \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n = -\boldsymbol{\mathcal{C}} \lambda \end{cases} \tag{273}$$

$$\begin{bmatrix} A & -\Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \\ \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) & \boldsymbol{\mathcal{C}} \end{bmatrix} \begin{bmatrix} \Delta \dot{\boldsymbol{q}} \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n \end{bmatrix} \tag{274}$$

Using the Schur complement (Equation 319):

$$\begin{aligned} \left(\boldsymbol{\mathcal{C}} + \Delta t^2 \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) A^{-1} \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n)^T \right) \lambda &= -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) \dot{\boldsymbol{q}}_n - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) A^{-1} b \\ &= -\delta(\boldsymbol{q}_n) - \Delta t \boldsymbol{\mathcal{H}}(\boldsymbol{q}_n) (\dot{\boldsymbol{q}}_n + \Delta \dot{\boldsymbol{q}}_{\text{free}}) \\ &\approx -\delta(\boldsymbol{q}_n + \Delta \boldsymbol{q}_{\text{free}}) = -\delta(\boldsymbol{q}_{\text{free}}) \end{aligned} \tag{275}$$

8.7 Models

8.7.1 Fixation

$$\delta(\boldsymbol{q}) = \boldsymbol{q} - \boldsymbol{q}_0 \tag{276}$$
$$\boldsymbol{\mathcal{H}}(\boldsymbol{q}) = \boldsymbol{I} \tag{277}$$
$$\widetilde{\boldsymbol{\mathcal{K}}} = \frac{\partial [\boldsymbol{\mathcal{H}}^T \lambda]}{\partial \boldsymbol{q}} = 0 \tag{278}$$

8.7.2 Bilteral

$$\delta(\boldsymbol{q}_1, \boldsymbol{q}_2) = \boldsymbol{q}_2 - \boldsymbol{q}_1 - \left(\boldsymbol{q}_{2_0} - \boldsymbol{q}_{1_0} \right) \tag{279}$$

$$
\begin{aligned}
\boldsymbol{\mathcal{H}}(\boldsymbol{q}_1, \boldsymbol{q}_2) &= \left[\tfrac{\partial \delta}{\partial \boldsymbol{q}_1} \quad \tfrac{\partial \delta}{\partial \boldsymbol{q}_2}\right] \\
&= [-\boldsymbol{I} \quad \boldsymbol{I}]
\end{aligned}
\tag{280}
$$

$$
\widetilde{\boldsymbol{\mathcal{K}}} = \frac{\partial[\boldsymbol{\mathcal{H}}^T \lambda]}{\partial \boldsymbol{q}} = 0 \tag{281}
$$

$$
\delta_{\text{free}} \tag{282}
$$

9 Mapping

A mapping is a coordinate transformation function $\boldsymbol{\mathcal{F}}$ such that:

$$\boldsymbol{q}_{\text{out}} = \boldsymbol{\mathcal{F}}(\boldsymbol{q}_{\text{in}}) \tag{283}$$

9.1 Velocity

The velocity is deduced from Equation 283:

$$\dot{\boldsymbol{q}}_{\text{out}} = \frac{d\boldsymbol{q}_{\text{out}}}{dt} = \frac{d\boldsymbol{\mathcal{F}}(\boldsymbol{q}_{\text{in}})}{dt} = \frac{d\boldsymbol{\mathcal{F}}(\boldsymbol{q}_{\text{in}})}{d\boldsymbol{q}_{\text{in}}}\frac{d\boldsymbol{q}_{\text{in}}}{dt} = \frac{d\boldsymbol{\mathcal{F}}(\boldsymbol{q}_{\text{in}})}{d\boldsymbol{q}_{\text{in}}}\dot{\boldsymbol{q}}_{\text{in}} \tag{284}$$

We introduce the jacobian matrix $\boldsymbol{\mathcal{J}}$ of the mapping:

$$\boldsymbol{\mathcal{J}}(\boldsymbol{q}) = \boldsymbol{\partial}\boldsymbol{\mathcal{F}}(\boldsymbol{q}) = \frac{\partial\boldsymbol{\mathcal{F}}(\boldsymbol{q})}{\partial\boldsymbol{q}} \tag{285}$$

Such that:

$$\dot{\boldsymbol{q}}_{\text{out}} = \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}} \tag{286}$$

9.2 Force

The power of the force applying on $\boldsymbol{q}_{\text{in}}$ is equivalent to the power of the force applying on $\boldsymbol{q}_{\text{out}}$:

$$\dot{\boldsymbol{q}}_{\text{in}}^T\boldsymbol{F}_{\text{in}}(\boldsymbol{q}_{\text{in}}) = \dot{\boldsymbol{q}}_{\text{out}}^T\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \tag{287}$$

Then,

$$\dot{\boldsymbol{q}}_{\text{in}}^T\boldsymbol{F}_{\text{in}}(\boldsymbol{q}_{\text{in}}) = (\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}})^T\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) = \dot{\boldsymbol{q}}_{\text{in}}^T\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \tag{288}$$

We can deduce from the principle of virtual work:

$$\boldsymbol{F}_{\text{in}}(\boldsymbol{q}_{\text{in}}) = \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \tag{289}$$

9.3 Derivatives

If we are interested in the derivatives, such as the stiffness matrix:

$$\begin{aligned}
\boldsymbol{\mathcal{K}}_{\text{in}}(\boldsymbol{q}_{\text{in}}) = \frac{\partial\boldsymbol{F}_{\text{in}}(\boldsymbol{q}_{\text{in}})}{\partial\boldsymbol{q}_{\text{in}}} &= \frac{\partial\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T}{\partial\boldsymbol{q}_{\text{in}}}\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\frac{\partial\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial\boldsymbol{q}_{\text{in}}} \\
&= \frac{\partial\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T}{\partial\boldsymbol{q}_{\text{in}}}\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\frac{\partial\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial\boldsymbol{q}_{\text{out}}}\frac{\partial\boldsymbol{q}_{\text{out}}}{\partial\boldsymbol{q}_{\text{in}}} \\
&= \frac{\partial\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T}{\partial\boldsymbol{q}_{\text{in}}}\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\boldsymbol{\mathcal{K}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\frac{\partial\boldsymbol{\mathcal{F}}(\boldsymbol{q}_{\text{in}})}{\partial\boldsymbol{q}_{\text{in}}} \\
&= \frac{\partial\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T}{\partial\boldsymbol{q}_{\text{in}}}\boldsymbol{F}_{\text{out}}(\boldsymbol{q}_{\text{out}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\boldsymbol{\mathcal{K}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})
\end{aligned} \tag{290}$$

The term $\frac{\partial\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T}{\partial\boldsymbol{q}_{\text{in}}}$ is called the geometric stiffness of the mapping.

The term $\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T\boldsymbol{\mathcal{K}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})$ is a projection of the matrix $\boldsymbol{\mathcal{K}}_{\text{out}}$ from the space “out” to the space “in”.

9.4 Mass

The kinetic energy:

$$\mathcal{T}_{\text{out}} = \frac{1}{2}\dot{\boldsymbol{q}}_{\text{out}}^T\boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\dot{\boldsymbol{q}}_{\text{out}} \tag{291}$$

From Equation 286:

$$\begin{aligned}\mathcal{T}_{\text{out}} &= \frac{1}{2}(\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})(\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}}) \\ &= \frac{1}{2}\dot{\boldsymbol{q}}_{\text{in}}^T \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}}\end{aligned} \tag{292}$$

We also have

$$\mathcal{T}_{\text{in}} = \frac{1}{2}\dot{\boldsymbol{q}}_{\text{in}}^T \boldsymbol{\mathcal{M}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}} \tag{293}$$

The kinetic energy is invariant under coordinate transformation: $\mathcal{T}_{\text{in}} = \mathcal{T}_{\text{out}}$. By identification, we can deduce that

$$\boldsymbol{\mathcal{M}}_{\text{in}}(\boldsymbol{q}_{\text{in}}) = \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}}) \tag{294}$$

9.5 Momentum

From Equation 11,

$$\begin{aligned}\boldsymbol{p}_{\text{in}} = \frac{\partial \mathcal{T}_{\text{in}}}{\partial \dot{\boldsymbol{q}}_{\text{in}}} &= \frac{\partial}{\partial \dot{\boldsymbol{q}}_{\text{in}}}\left(\frac{1}{2}\dot{\boldsymbol{q}}_{\text{in}}^T \boldsymbol{\mathcal{M}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}}\right) \\ &= \boldsymbol{\mathcal{M}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}} \\ &= \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}}\end{aligned} \tag{295}$$

From Equation 286:

$$\boldsymbol{p}_{\text{in}} = \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\dot{\boldsymbol{q}}_{\text{out}} \tag{296}$$

We also have:

$$\begin{aligned}\boldsymbol{p}_{\text{out}} = \frac{\partial \mathcal{T}_{\text{out}}}{\partial \dot{\boldsymbol{q}}_{\text{out}}} &= \frac{\partial}{\partial \dot{\boldsymbol{q}}_{\text{out}}}\left(\frac{1}{2}\dot{\boldsymbol{q}}_{\text{out}}^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\dot{\boldsymbol{q}}_{\text{out}}\right) \\ &= \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})\dot{\boldsymbol{q}}_{\text{out}}\end{aligned} \tag{297}$$

We can deduce that:

$$\boldsymbol{p}_{\text{in}} = \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{p}_{\text{out}} \tag{298}$$

9.6 Newton's Second Law of Motion

In Section 2.1, we deduced the Newton's second law of motion from the Euler-Lagrange equation (Equation 21):

$$\boldsymbol{\mathcal{M}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\ddot{\boldsymbol{q}}_{\text{in}(t)} + \boldsymbol{\mathcal{C}}(\boldsymbol{q}_{\text{in}}, \dot{\boldsymbol{q}}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}(t)} = \boldsymbol{F}_{\text{in}}(\boldsymbol{q}_{\text{in}}, \dot{\boldsymbol{q}}_{\text{in}}) \tag{299}$$

We are already able to compute the inertia term ($\boldsymbol{\mathcal{M}}_{\text{in}} = \boldsymbol{\mathcal{J}}^T \boldsymbol{\mathcal{M}}_{\text{out}}\boldsymbol{\mathcal{J}}$ in Equation 294) and the forces ($\boldsymbol{F}_{\text{in}} = \boldsymbol{\mathcal{J}}\boldsymbol{F}_{\text{out}}$ in Equation 289), so let's focus on the Coriolis term:

$$\boldsymbol{\mathcal{C}}(\boldsymbol{q}_{\text{in}}, \dot{\boldsymbol{q}}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}(t)} = \dot{\boldsymbol{\mathcal{M}}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}(t)} - \frac{1}{2}\dot{\boldsymbol{q}}_{\text{in}}(t)^T \frac{\partial \boldsymbol{\mathcal{M}}_{\text{in}}}{\partial \boldsymbol{q}_{\text{in}}}\dot{\boldsymbol{q}}_{\text{in}(t)} \tag{300}$$

First term:

$$\begin{aligned}\dot{\boldsymbol{\mathcal{M}}}_{\text{in}}(\boldsymbol{q}_{\text{in}})\dot{\boldsymbol{q}}_{\text{in}(t)} &= \frac{d\boldsymbol{\mathcal{M}}_{\text{in}}}{dt}\dot{\boldsymbol{q}}_{\text{in}} \\ &= \frac{d}{dt}[\boldsymbol{\mathcal{J}}^T \boldsymbol{\mathcal{M}}_{\text{out}}\boldsymbol{\mathcal{J}}]\dot{\boldsymbol{q}}_{\text{in}} \\ &= \dot{\boldsymbol{\mathcal{J}}}^T \boldsymbol{\mathcal{M}}_{\text{out}}\boldsymbol{\mathcal{J}}\dot{\boldsymbol{q}}_{\text{in}} + \boldsymbol{\mathcal{J}}^T \dot{\boldsymbol{\mathcal{M}}}_{\text{out}}\boldsymbol{\mathcal{J}}\dot{\boldsymbol{q}}_{\text{in}} + \boldsymbol{\mathcal{J}}^T \boldsymbol{\mathcal{M}}_{\text{out}}\dot{\boldsymbol{\mathcal{J}}}\dot{\boldsymbol{q}}_{\text{in}}\end{aligned} \tag{301}$$

The second term involve the derivative of the mass with respect to the state:

$$
\begin{aligned}
\frac{\partial \boldsymbol{\mathcal{M}}_{\text{in}}}{\partial \boldsymbol{q}_{\text{in}}} &= \frac{\partial \left[\boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}}) \right]}{\partial \boldsymbol{q}_{\text{in}}} \\
&= \frac{\partial \boldsymbol{\mathcal{J}}^T}{\partial \boldsymbol{q}_{\text{in}}} \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \frac{\partial \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial \boldsymbol{q}_{\text{in}}} \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}}) + \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})^T \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}}) \frac{\partial \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})}{\partial \boldsymbol{q}_{\text{in}}}
\end{aligned}
\tag{302}
$$

The term $\frac{\partial \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial \boldsymbol{q}_{\text{in}}}$:

$$
\begin{aligned}
\frac{\partial \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial \boldsymbol{q}_{\text{in}}} &= \frac{\partial \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial \boldsymbol{q}_{\text{out}}} \frac{\partial \boldsymbol{q}_{\text{out}}}{\partial \boldsymbol{q}_{\text{in}}} \\
&= \frac{\partial \boldsymbol{\mathcal{M}}_{\text{out}}(\boldsymbol{q}_{\text{out}})}{\partial \boldsymbol{q}_{\text{out}}} \boldsymbol{\mathcal{J}}(\boldsymbol{q}_{\text{in}})
\end{aligned}
\tag{303}
$$

10 Maths

10.1 Outer Product

Given two vectors of size $m \times 1$ and $n \times 1$ respectively $u = (u_1, ..., u_n)$, $v = (v_1, ..., v_n)$, their outer product, denoted $u \otimes v$, is defined as the $m \times n$ matrix A obtained by multiplying each element of u by each element of v:

$$u \otimes v = A = \begin{bmatrix} u_1v_1 & u_1v_2 & \dots & u_1v_n \\ u_2v_1 & u_2v_2 & \dots & u_2v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_mv_1 & u_mv_2 & \dots & u_mv_n \end{bmatrix} \tag{304}$$

The outer product $u \otimes v$ is equivalent to a matrix multiplication uv^T.

10.2 Derivative of the 2-norm

The 2-norm of vector $x = (x_1, ..., x_n)$ is

$$\|x\|_2 := \sqrt{\sum_{i=1}^{n} x_i^2} \tag{305}$$

The partial derivative of the 2-norm is given by

$$\frac{\partial}{\partial x_k} \|x\|_2 = \frac{x_k}{\|x\|_2} \tag{306}$$

The derivative with respect to x is

RESULT

$$\frac{\partial \|x\|_2}{\partial x} = \frac{x}{\|x\|_2} \tag{307}$$

Result can be found in [2].

Considering two points a and b, and $\gamma = a - b$:

$$\begin{aligned} \frac{\partial \|a-b\|}{\partial a} &= \frac{\partial \|\gamma\|}{\partial \gamma} \cdot \frac{\partial \gamma}{\partial a} \\ &= \frac{\gamma}{\|\gamma\|_2} \cdot 1 \\ &= \frac{a-b}{\|a-b\|_2} \end{aligned} \tag{308}$$

and

$$\frac{\partial \|a-b\|}{\partial a} = \frac{b-a}{\|b-a\|_2} \tag{309}$$

10.3 Derivative of a normalized vector

The normalized vector of x is a vector in the same direction but with norm 1. It is denoted $\hat{x}$ and given by

$$\hat{x} = \frac{x}{\|x\|_2} \tag{310}$$

Using the quotient rule, the partial derivative of the normalized vector is given by

$$\frac{\partial \hat{x}}{\partial x} = \frac{\|x\|_2 \frac{\partial x}{\partial x} - x \frac{\partial \|x\|_2}{\partial x}}{\|x\|_2^2} \tag{311}$$

Using Equation 307,

$$\frac{\partial \hat{x}}{\partial x} = \frac{\|x\|_2 I - x \frac{x}{\|x\|_2}}{\|x\|_2^2} \tag{312}$$

Finally,

RESULT

$$\frac{\partial \hat{x}}{\partial x} = \frac{1}{\|x\|_2} I - \frac{1}{\|x\|_2^3} x \otimes x \tag{313}$$

Considering two points a and b, and $\gamma = a - b$:

$$\begin{aligned} \frac{\partial \widehat{a-b}}{\partial a} = \frac{\partial \hat{\gamma}}{\partial a} &= \frac{\partial \hat{\gamma}}{\partial \gamma} \cdot \frac{\partial \gamma}{\partial a} \\ &= \frac{1}{\|\gamma\|_2} I - \frac{1}{\|\gamma\|_2^3} \gamma \otimes \gamma \end{aligned} \tag{314}$$

$$\begin{aligned} \frac{\partial \widehat{a-b}}{\partial b} = \frac{\partial \hat{\gamma}}{\partial b} &= \frac{\partial \hat{\gamma}}{\partial \gamma} \cdot \frac{\partial \gamma}{\partial b} \\ &= -\frac{1}{\|\gamma\|_2} I + \frac{1}{\|\gamma\|_2^3} \gamma \otimes \gamma \\ &= -\frac{\partial \widehat{a-b}}{\partial a} \end{aligned} \tag{315}$$

10.4 Schur Complement

The following is a linear system of equations in the matrix form using a 2x2 partition:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \tag{316}$$

Suppose p, q are nonnegative integers such that $p + q > 0$, and suppose A, B, C, D are respectively $p \times p$, $p \times q$, $q \times p$, and $q \times q$ matrices.

$$\begin{cases} Ax + By = u \\ Cx + Dy = v \end{cases} \tag{317}$$

Using the first line, we can express x in terms of y:

$$x = A^{-1}(u - By) \tag{318}$$

Substituting this expression into the second line of the equation:

$$(D - CA^{-1}B)y = v - CA^{-1}u \tag{319}$$

$(D - CA^{-1}B)$ is the Schur complement of the block A.

Similarly, we can express y in terms of x using the first line:

$$y = B^{-1}(u - Ax) \tag{320}$$

Substituting this expression into the second line of the equation:

$$(C - DB^{-1}A)x = v - DB^{-1}u \tag{321}$$

10.5 Integration by parts

$$
\begin{aligned}
\int_a^b u(x)v'(x)\ dx &= [u(x)v(x)]_a^b - \int_a^b u'(x)v(x)\ dx \\
&= u(b)v(b) - u(a)v(a) - \int_a^b u'(x)v(x)\ dx
\end{aligned}
\tag{322}
$$

11 Other Resources

[3]

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