Spatial & Generalized Coordinate System

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1 Introduction

Spatial Coordinates can be termed as Cartesian coordinates, in which problem is generally provided to us. When there is a holonomic constraint, which creates a restriction in coordinates; our degrees of freedom are reduced by the constraint equation present to us. That is where generalized coordinates play its role. The mechanical problem become much easier to visualize and solve, when such a transformation can occur explicitly of spatial coordinates to generalized coordinates. The coordinates of latter system is independent and thus no requirement of constraint equation is required. However, if such an explicit transformation is unable to happen, we can still solve the problem using method of multipliers. In this document we shall see the implementation of Principle of Least Constraint solving simple mechanical problems of a simple pendulum as well as a diatomic molecule, using both spatial as well as generalized coordinate. Thus, an effort is made to visualize the change of Forces and masses when the coordinates are transformed in such a way.

2 Simple Pendulum Problem Introduction

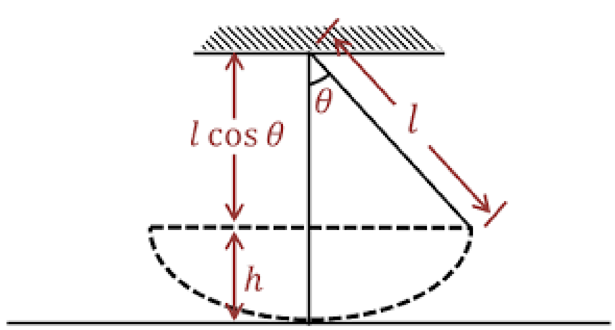

Figure 1: Simple Pendulum

First let us try out the problem without any transformation,i.e; considering Cartesian coordinates (x, y). Let us consider hinged point as our origin.
Force in x-direction is 0 and in y-direction is $-mg$, thus force vector becomes:

$$\mathbf{F}^T = \begin{bmatrix} 0 & -mg \end{bmatrix}$$

Constraint Equation: $x^2 + y^2 = l^2$
Differentiating twice with respect to time to obtain the equation in the general form of $\mathbf{n}^T\ddot{\mathbf{r}} = s$:

$\Big[$**NOTE**: In general, the constrained equation is of the form $\mathbf{n}^T\ddot{\mathbf{q}} = s$, but since we are not transforming our coordinates here, we will focus on above mentioned equation.$\Big]$

$$\begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} \ddot{x} \\ \ddot{y} \end{bmatrix} = -(\dot{x}^2 + \dot{y}^2) \tag{1}$$

Now, here $\mathbf{n}$ is $\mathbf{r} = \begin{bmatrix} x & y \end{bmatrix}^T$ and $s = -(\dot{x}^2 + \dot{y}^2)$
Now, by the Principle of Least Constraint:

$$\delta(G + \alpha C) = 0$$

where α is multiplier, and C represents constrained equation.

$$\delta\left(\frac{\sum_{k=1}^{N} m_k |\frac{d^2 r_k}{dt^2} - \frac{F_k}{m_k}|^2}{2} + \alpha(\mathbf{n}\ddot{\mathbf{r}} - s)\right) = 0$$

Taking variation with free parameters $\ddot{r}_i$, here $\ddot{x}$ and $\ddot{y}$, we get;

$$\sum_i (m\ddot{r}_i - F_i + \alpha n_i)\delta\ddot{r}_i = 0$$

NOTE: $\delta\ddot{r}_i = \frac{1}{2}\delta r_i t^2$, where δr_i are virtual displacement that are arbitrary. This gives the value of each of their coefficient as 0 and thus,

$$m\ddot{r}_i = F_i - \alpha n_i \tag{2}$$

or in vector format;

$$m\ddot{\mathbf{r}} = \mathbf{F} - \alpha\mathbf{n} \tag{3}$$

Eq. (2) and Eq. (3) is the famous Principle of Least Constraint use for solving mechanical problems with holonomic as well as some non-holonomic constraints. Thus taking dot product with $\mathbf{n}$ in above equation and then using it with constrained equation will give us the value of $\alpha = \frac{\mathbf{n^T}.\mathbf{F} - ms}{\mathbf{n^T}.\mathbf{n}}$
Therefore, in this problem, $\alpha = \frac{-mgy + m\dot{x}^2 + m\dot{y}^2}{l^2}$

Thus, we get by Eq. (3) as;

$$m\begin{bmatrix}\ddot{x}\\ \ddot{y}\end{bmatrix} = \begin{bmatrix}0\\ -mg\end{bmatrix} - \frac{-mgy + m\dot{x}^2 + m\dot{y}^2}{l^2}\begin{bmatrix}x\\ y\end{bmatrix}$$

Now, if we write $x = lsin(\theta)$ and $y = -lcos(\theta)$, solving both the above equation will individually give us;

$$\ddot{\theta} = -\frac{g}{l}sin(\theta)$$

Now, we will see the power of generalized coordinates, which here we take as polar coordinates. Now, our constrained equation is giving us: $\ddot{r} = 0$ and we know that variation of r is not possible.

Now, we know that our constrained is embedded in transformation. To show this practically, we will solve problem once, by not taking contribution from C (no work will be done by holonomic constrained force) and then again we will solve by above shown method but in our generalized polar coordinates.

So,

$$\delta G = 0;$$

$$\frac{\partial G}{\partial \ddot{\theta}}(\delta\ddot{\theta} \equiv \delta\theta) = 0$$

$$\frac{\partial G}{\partial \ddot{x}}\Big(\frac{\partial x}{\partial \theta} \equiv \frac{\partial \ddot{x}}{\partial \ddot{\theta}}\Big) + \frac{\partial G}{\partial \ddot{y}}\Big(\frac{\partial y}{\partial \theta} \equiv \frac{\partial \ddot{y}}{\partial \ddot{\theta}}\Big) = 0$$

$$m\ddot{x}\frac{\partial x}{\partial \theta} + m(\ddot{y} + g)\frac{\partial y}{\partial \theta} = 0$$

Now, we can use $x = lsin(\theta)$ and $y = -lcos(\theta)$, and thus we will get the same final answer as;

$$\ddot{\theta} = -\frac{g}{l}sin(\theta)$$

Now, we shall see the implementation of constraint equation with generalized coordinates ($q1 = r$ and $q2 = \theta$) as well:

$$\begin{bmatrix}1 & 0\end{bmatrix}\begin{bmatrix}\ddot{r}\\ \ddot{\theta}\end{bmatrix} = 0$$

Here, the constrained equation is in the desired form of $\mathbf{n}.\ddot{\mathbf{q}} = s$, where $n = \begin{bmatrix}1 & 0\end{bmatrix}^T$ and $s = 0$. Now, here the force vector will also be transformed. Let me use f for representing force in this system.

We can use the generalized formula for transformed force as:

$$f_i = \sum_j F_j \frac{\partial r_j}{\partial q_i}$$

which will give us $f_r = mgcos(\theta)$ and $f_\theta = -mgsin(\theta)$.
The mass for generalized coordinate can be calculated by any one formula of $\sum_k m_k \frac{\partial \ddot{r}_k}{\partial \ddot{q}_i} = m_i^{'} \ddot{q}_i$ or by Kinetic Energy one of: $\sum_k \frac{1}{2} m_k \dot{r}_k^2 = \sum_i \frac{1}{2} m_i^{'} \dot{q}_i^2$, which will give us:

$$m_\theta = ml^2 \tag{4}$$

Now,

$$G = \frac{1}{2}\left(\left(\ddot{r} - \frac{mgcos(\theta)}{m}\right)^2 + (\ddot{\theta} - \frac{-mgsin(\theta)}{ml^2})\right)$$

Therefore; $\delta(G + \alpha C) = 0$

$$\delta\left(\frac{1}{2}\left(\left(\ddot{r} - \frac{mgcos(\theta)}{m}\right)^2 + (\ddot{\theta} - \frac{-mgsin(\theta)}{ml^2})\right) + \alpha(\mathbf{n}.\ddot{\mathbf{q}})\right) = 0$$

This give again the similar expression in generalized coordinate:

$$M\ddot{\mathbf{q}} = \mathbf{f} - \alpha \mathbf{n}$$

Now, $\alpha = \frac{\mathbf{n^T}.\mathbf{f}}{\mathbf{n^T}.\mathbf{n}} = mgcos(\theta)$. Thus we get;

$$m_i \ddot{q}_i = f_i - \alpha n_i$$

Thus we get, $\ddot{r} = 0$ and $\ddot{\theta} = -\frac{g}{l} sin(\theta)$

3 Diatomic Molecule

Let us try to solve a more complex problems in similar ways; Let us assume

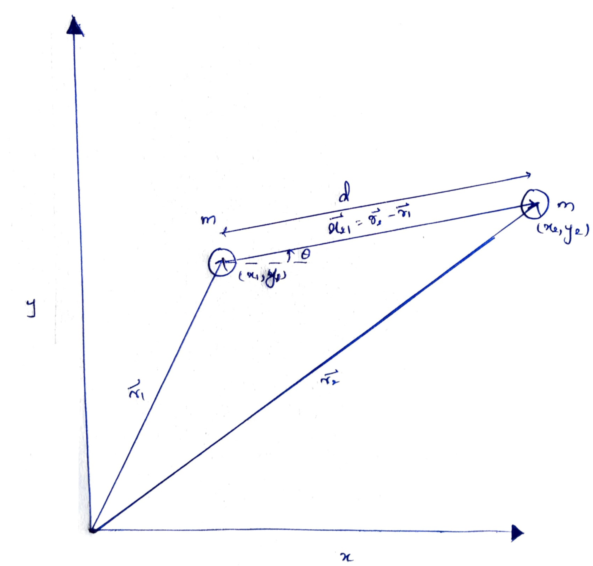

Figure 2: Diatomic Molecule Particles

that mass of both the particles are same for simplicity:

The constraint of the problem restricts the change in length between the particles, thus, constrained equation becomes:

$$(x_1 - x_2)^2 + (y_1 - y_2)^2 = d^2$$

Differentiating twice with respect to time,

$$\begin{bmatrix}(x_1 - x_2) & (y_1 - y_2) & -(x_1 - x_2) & -(y_1 - y_2)\end{bmatrix} \begin{bmatrix}\ddot{x}_1 \\ \ddot{y}_1 \\ \ddot{x}_2 \\ \ddot{y}_2\end{bmatrix} = -((\dot{x}_1 - \dot{x}_2)^2 + (\dot{y}_1 - \dot{y}_2)^2)$$

Force vector: $F = \begin{bmatrix}F_x1 & F_y1 & F_x2 & F_y2\end{bmatrix}^T$

$$\alpha = \frac{\mathbf{n}^T.\mathbf{F} - ms}{\mathbf{n^T}.\mathbf{n}} = \frac{(F_x1 - F_x2)(x_1 - x_2) + (F_y1 - F_y2)(y_1 - y_2) + m((\dot{x}_1 - \dot{x}_2)^2 + (\dot{y}_1 - \dot{y}_2)^2)}{2d^2}$$

Thus, we get our equation of motion from $m\ddot{r}_i = F_i - \alpha n_i$ as:

$$m\ddot{x}_1 = F_x1 - \alpha(x_1 - x_2)$$

$$m\ddot{y}_1 = F_y1 - \alpha(y_1 - y_2)$$
$$m\ddot{x}_2 = F_x2 + \alpha(x_1 - x_2)$$
$$m\ddot{y}_2 = F_y2 + \alpha(y_1 - y_2)$$

We can see that here, our generalized coordinates can be (x_1, y_1, θ). The transformation embeds the constraint equation.
We can use the transformation: $x_2 = x_1 + dcos(\theta)$ and $y_2 = y_1 + dsin(\theta)$
By using above transformation, above equations of motion will yield us equation of motion in generalized coordinates as:

$$m\ddot{x}_1 = F_x1 + \frac{cos(\theta)}{2}\Big(cos(\theta)(F_x2 - F_x1) + sin(\theta)(F_y2 - F_y1) + md\dot{\theta}^2\Big)$$

$$m\ddot{y}_1 = F_y1 + \frac{sin(\theta)}{2}\Big(cos(\theta)(F_x2 - F_x1) + sin(\theta)(F_y2 - F_y1) + md\dot{\theta}^2\Big)$$

These two will be same, but 3rd and 1st equation as well as 2nd and 4th equation will individually yield:

$$md\ddot{\theta} = (F_y2 - F_y1)cos(\theta) - (F_x2 - F_x1)sin(\theta)$$

Thus, now we have to prove that by taking variation of G with respect to our generalize coordinates can also derive our above three equations of motion.
G in terms of spatial coordinates is:

$$G = \frac{1}{2}\Bigg(\big(\ddot{x}_1 - \frac{F_x1}{m}\big)^2 + \big(\ddot{y}_1 - \frac{F_y1}{m}\big)^2 + \big(\ddot{x}_2 - \frac{F_x2}{m}\big)^2 + \big(\ddot{y}_2 - \frac{F_y2}{m}\big)^2\Bigg)$$

Now,

$$\delta G = \sum_j \frac{\partial G}{\partial \ddot{q}_j}\delta\ddot{q}_j = \sum_j\sum_i \frac{\partial G}{\partial \ddot{r}_i}\frac{\partial r_i}{\partial q_j}(\delta\ddot{q}_j \equiv \delta q_j) = 0$$

Since, δq_j are virtual displacement and thus arbitrary, therefore, for all js

$$\sum_i \frac{\partial G}{\partial \ddot{r}_i}\frac{\partial r_i}{\partial q_j} = 0$$

Taking $q_1 = x_1$,

$$\frac{\partial G}{\partial \ddot{x}_1} + \frac{\partial G}{\partial \ddot{x}_2}\frac{\partial x_2}{\partial x_1} = 0$$

Hence,

$$\frac{\partial G}{\partial \ddot{x}_1} + \frac{\partial G}{\partial \ddot{x}_2} = 0$$

$$\ddot{x}_1 + \ddot{x}_2 - \frac{F_x1 + F_x2}{m} = 0$$

which gives us,

$$2\ddot{x}_1 - dsin(\theta)\ddot{\theta} - dcos(\theta)\dot{\theta}^2 - \frac{F_x1 + F_x2}{m} = 0$$

Similarly for, $q_2 = y_1$, we get;

$$2\ddot{y}_1 + dcos(\theta)\ddot{\theta} - dsin(\theta)\dot{\theta}^2 - \frac{F_y1 + F_y2}{m} = 0$$

For the $q_3 = \theta$, we will get;

$$-(\ddot{x}_2 - \frac{F_x2}{m})sin(\theta) + (\ddot{y}_2 - \frac{F_y2}{m})cos(\theta) = 0 \tag{5}$$

which gives us;

$$\ddot{y}_1 cos(\theta) - \ddot{x}_1 sin(\theta) + d\ddot{\theta} + \frac{F_x2sin(\theta) - F_y2cos(\theta)}{m} = 0$$

Multiplying 2nd equation with $sin(\theta)$ and then subtracting 1st equation multiplied with $cos(\theta)$;

$$2(\ddot{y}_1 cos(\theta) - \ddot{x}_1 sin(\theta)) + d\ddot{\theta} - \frac{-(F_y1 + F_y2)cos(\theta) + (F_x1 + F_x2)sin(\theta)}{m} = 0$$

Using $\ddot{y}_1 cos(\theta) - \ddot{x}_1 sin(\theta)$ value in third equation:

$$-\frac{d\ddot{\theta} + \frac{-(F_y1+F_y2)cos(\theta)+(F_x1+F_x2)sin(\theta)}{m}}{2} + d\ddot{\theta} + \frac{F_x2sin(\theta) - F_y2cos(\theta)}{m} = 0$$

This finally gives us,

$$\ddot{\theta} = \frac{-(F_x2 - F_x1)sin(\theta) + (F_y2 - F_y1)cos(\theta)}{md} = 0$$

Using this value in first and second equation will finally give us same expression of $\ddot{x}_1$ and $\ddot{y}_1$

We were able to do so, because the constraint force do no work!

Let's see the relation of Principle of Least Constraint and Least Action in such cases considered where the Holonomic Constraints are embedded in transformation:

$$\sum_j \frac{\partial G}{\partial \ddot{q}_j} \delta \ddot{q}_j = 0 \tag{6}$$

Now,

$$\sum_j \sum_i \Big(\frac{\partial G}{\partial \ddot{r}_i} \frac{\partial \ddot{r}_i}{\partial \ddot{q}_j} \Big) \delta \ddot{q}_j = 0$$

From calculus of variation, we can say that: $\frac{\partial \ddot{r}_i}{\partial \ddot{q}_j} = \frac{\partial r_i}{\partial q_j}$, and $(1/2)\delta \ddot{q}_j dt^2 = \delta q_j$:

$$\sum_j \sum_i \Big(\frac{\partial G}{\partial \ddot{r}_i} \frac{\partial r_i}{\partial q_j} \Big) \delta q_j = 0$$

And Then;

$$\sum_i (m_i \ddot{r}_i - F_i)\frac{\partial r_i}{\partial q_j} = 0$$

After integration of parts, it gives us:

$$\sum_i [\frac{d}{dt} m_i \dot{r}_i \frac{\partial r_i}{\partial q_j} - m_i \dot{r}_i \frac{d}{dt}\Big(\frac{\partial r_i}{\partial q_j}\Big) - (-\frac{\partial V_i}{\partial r_i}\frac{\partial r_i}{\partial q_j})] = 0 \tag{7}$$

Again,we know that

$$\frac{d}{dt}\Big(\frac{\partial r_i}{\partial q_j}\Big) = \frac{\partial \dot{r}_i}{\partial q_j} = \frac{\partial v_i}{\partial q_j}$$

where, v_i represents spatial velocity, and,

$$\frac{\partial v_i}{\partial \dot{q}_j} = \frac{\partial r_i}{\partial q_j}$$

the original working equation (6) from these substitution comes out to be..

$$\sum_i (\frac{d}{dt}(m_i v_i \frac{\partial v_i}{\partial \dot{q}_j}) - m_i v_i (\frac{\partial v_i}{\partial q_j}) + (\frac{\partial V_i}{\partial q_j})) = 0$$

$$\sum_i (\frac{d}{dt}\frac{\partial \frac{m_i v_i^2}{2}}{\partial \dot{q}_j} - \frac{\partial \frac{m_i v_i^2}{2}}{\partial q_j} + \frac{\partial V_i}{\partial q_j}) = 0 \tag{8}$$

Therefore:

$$[\frac{d}{dt}(\frac{\partial T}{\partial \dot{q}_j}) - \frac{\partial (T-V)}{\partial q_j}] = 0 \tag{9}$$

If V(potential energy) is independent of the velocity then the derived equation is generalized in Lagrangian form: L = T - V :

$$[\frac{d}{dt}(\frac{\partial L}{\partial \dot{q}_j}) - \frac{\partial L}{\partial q_j}] = 0 \tag{10}$$

Now, by inverse Legendre's Transformation, we can derive the Hamiltonian of the system as well:

$$H = \sum_k \dot{q}_k p_k - L$$

We know that, we have replace $T - V$ as L in spatial coordinates. So,

$$L = \frac{1}{2}m\Bigg(\dot{x}_1^2 + \dot{y}_1^2 + \dot{x}_2^2 + \dot{y}_2^2\Bigg) + \Bigg(x_1 F_x 1 + y_1 F_y 1 + x_2 F_x 2 + y_2 F_y 2\Bigg)$$

Let us now apply the equation for generalized momentum on Lagrangian, that is;

$$\frac{\partial L}{\partial \dot{q}_i} = p_i$$

For, $q_1 = x_1$, we get;

$$p_1 = m\dot{x}_1 + m\dot{x}_2 \frac{\partial \dot{x}_2}{\partial \dot{x}_1} = m(\dot{x}_1 + \dot{x}_2)$$

Similarly for $q_1 = y_1$, we get;

$$p_2 = m(\dot{y}_1 + \dot{y}_2)$$

For, $q_3 = \theta$, we proceed as;

$$p_3 = \frac{\partial L}{\partial \dot{\theta}}$$

$$p_3 = \frac{m}{2} \frac{\partial(\dot{x}_2^2 + \dot{y}_2^2)}{\partial \dot{\theta}}$$

$$p_3 = m(\dot{x}_2 \frac{\partial \dot{x}_2}{\partial \theta} + \dot{y}_2 \frac{\partial \dot{y}_2}{\partial \theta})$$

$$p_3 = md(-\dot{x}_2 sin(\theta) + \dot{y}_2 cos(\theta)) \tag{11}$$

Now, let us verify the equation of Hamiltonian for derivative of momentum, that is;

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

Verifying for the first variable,

$$m(\ddot{x}_1 + \ddot{x}_2) = F_x 1 + F_x 2 \frac{\partial x_2}{\partial x_1} = F_x 1 + F_x 2$$

which is true! Now, similar will be the case for second variable;

$$m(\ddot{y}_1 + \ddot{y}_2) = F_y 1 + F_y 2 \frac{\partial y_2}{\partial y_1} = F_y 1 + F_y 2$$

Now, for third variable $q_3 = \theta$, we get,

$$\frac{dp_3}{dt} = \dot{\theta} \frac{p_3}{\partial \theta} + \frac{\partial(F_x 2 x_2 + F_y 2 y_2)}{\partial \theta}$$

Solving LHS (using Eq. (11)) and RHS for the verification;

$$md(-\ddot{x}_2 sin(\theta) + \ddot{y}_2 cos(\theta) - \dot{x}_2 cos(\theta)\dot{\theta} - \dot{y}_2 sin(\theta)\dot{\theta}) = md(-\dot{x}_2 cos(\theta) - \dot{y}_2 sin(\theta)) - d(F_x 2 sin(\theta) - F_y 2 cos(\theta))$$

This gives us Eq.(5) on solving and hence verified:

$$m(-\ddot{x}_2 sin(\theta) + \ddot{y}_2 cos(\theta)) = -F_x 2 sin(\theta) + F_y 2 cos(\theta)$$

Additional, Legendre Transformation equation is obvious:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

as, $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ is independent of p_i. If expressed in spatial coordinates, H can be expanded as:

$$H = \frac{1}{2}m\Bigg(\dot{x}_1^2 + \dot{y}_1^2 + \dot{x}_2^2 + \dot{y}_2^2\Bigg) - \Bigg(x_1 F_x 1 + y_1 F_y 1 + x_2 F_x 2 + y_2 F_y 2\Bigg)$$