Resolving Torques in Rigid Multicentred Molecules

W. Smith

The purpose of this note is to resolve the problem that arises in simulating rigid multicentred molecules, where the 'centres' are not necessarily simple atoms, but may be complicated entities such as a multipoles, which themselves experience torques in addition to simple site forces. The problem is how to exploit these torques in computing the dynamics of the molecule as a whole.

We begin with the simplest case, a set of point particles $\{i : i = 1, \ldots, N\}$ arranged in a rigid framework. It is assumed that each particle is subjected to a force $\mathbf{F}_i$. What is the torque of the system about an arbitrary point?

If each particle is located at a point $\mathbf{R}_i$ defined with respect to an arbitrary origin $\mathbf{O}$, the torque *about the centre of mass* of the system ($\mathbf{T}_c$) is given by:

$$\mathbf{T}_c = \sum_{i=1}^{N} (\mathbf{R}_i - \mathbf{R}_c) \times \mathbf{F}_i \tag{1}$$

where the centre of mass $\mathbf{R}_c$ is given by:

$$\mathbf{R}_c = \frac{1}{M} \sum_{i=1}^{N} m_i \mathbf{R}_i \tag{2}$$

with

$$M = \sum_{i=1}^{N} m_i \tag{3}$$

being the total mass of the system.

Equation (1) can be expanded as follows:

$$\mathbf{T}_c = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \sum_{i=1}^{N} \mathbf{R}_c \times \mathbf{F}_i$$

$$\mathbf{T}_c = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \mathbf{R}_c \times \mathbf{F}_c$$

where

$$\mathbf{F}_c = \sum_{i=1}^{N} \mathbf{F}_i \tag{4}$$

is the sum of the forces acting on the whole system. Hence:

$$\sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i = \mathbf{T}_c + \mathbf{R}_c \times \mathbf{F}_c$$

or

$$\mathbf{T}_o = \mathbf{T}_c + \mathbf{R}_c \times \mathbf{F}_c \tag{5}$$

where

$$\mathbf{T}_o = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i \tag{6}$$

is the torque about the arbitrary point $\mathbf{O}$

Thus for this case we arrive at a simple rule: *The torque of a system about an arbitrary point is the the sum of the torque about the centre of mass and the torque due to the net force acting on the centre of mass of the system.*

A more complicated case arises when each point particle is replaced by some other entity, such as a small, rigid cluster of points (i.e. a compound particle), which experiences a torque in addition to the net force acting on it. How are these forces and torques to be combined into a total torque for the full assembly?

We begin with the compound particles. Each has a torque about its centre of mass $\mathbf{T}_n$ which we can write as:

$$\mathbf{T}_n = \sum_{i=1}^{P_n} (\mathbf{R}_i - \mathbf{R}_n) \times \mathbf{F}_i \tag{7}$$

where the centre of mass $\mathbf{R}_n$ is of course given by:

$$\mathbf{R}_n = \frac{1}{M_n} \sum_{i=1}^{P_n} m_i \mathbf{R}_i \tag{8}$$

with the total mass of the compound particle being:

$$M_n = \sum_{i=1}^{P_n} m_i \tag{9}$$

The vectors $\mathbf{R}_i$ are again specified with respect to an arbitrary origin $\mathbf{O}$

Once again, we may expand this expression to give:

$$\mathbf{T}_n = \sum_{i=1}^{P_n} \mathbf{R}_i \times \mathbf{F}_i - \sum_{i=1}^{P_n} \mathbf{R}_n \times \mathbf{F}_i$$

and we can form the vector sum ($\mathbf{T}_P$) of all such torques for the entire system (P being the number of compound particles):

$$\mathbf{T}_P = \sum_{n=1}^{P} \mathbf{T}_n = \sum_{n=1}^{P}\sum_{i=1}^{P_n} \mathbf{R}_i \times \mathbf{F}_i - \sum_{n=1}^{P}\sum_{i=1}^{P_n} \mathbf{R}_n \times \mathbf{F}_i$$

or

$$\mathbf{T}_P = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i - \sum_{n=1}^{P} \mathbf{R}_n \times \mathbf{F}_n \tag{10}$$

where we have simply expanded the double summation in the first term on the right, so that $N = \sum_{n=1}^{P} P_n$, and where $\mathbf{F}_n$ represents the net force acting on each compound particle i.e.

$$\mathbf{F}_n = \sum_{i=1}^{P_n} \mathbf{F}_i$$

Equation (10), with a little rearrangement, may be rewritten as:

$$\mathbf{T}_o = \mathbf{T}_P + \sum_{n=1}^{P} \mathbf{R}_n \times \mathbf{F}_n \tag{11}$$

where

$$\mathbf{T}_o = \sum_{i=1}^{N} \mathbf{R}_i \times \mathbf{F}_i \tag{12}$$

is once again the total torque of the system about the arbitrary point $\mathbf{O}$. The equation (11) has an obvious physical interpretation: *The net torque of a rigid system about an arbitrary point* $\mathbf{O}$ *is the vector sum of all the torques* $\mathbf{T}_n$ *acting on individual sites plus the sum of the torques arising from the net force* $\mathbf{F}_n$ *on each site acting about the point* $\mathbf{O}$. (It should be apparent that this follows logically from the rule given in the previous simple case.)

It should be noted that this result will hold, even if the 'arbitrary' point is the centre of mass of the whole system. It will also apply if the compound particles are replaced by equivalent point particles possessing multipolar attributes, such as point dipoles and quadrupoles.