RIGID pIB METHOD WITH A NEUTRALLY BUOYANT RIGID BODY

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In the rigid pIB method [1], a rigid body is connected to a fluid in which it is immersed by a system of stiff, zero-rest-length springs. In the equation of motion of the body, the relevant mass density of the body is its *excess* mass density, i.e. the difference between the density of the body and the density of the fluid. The reason for this is that fluid is everywhere in the IB method; it does not just surround the body but actually coexists in the same space with the body, and within that space the fluid is effectively constrained to move rigidly along with the body by the aforementioned stiff springs. Thus the fluid already accounts for a certain amount of mass, and the body need only account for the excess. We are concerned here, however, with the situation in which there is no excess, and the body is then said to be neutrally buoyant.

In its equation of motion, the body then appears as a massless object, and likewise it has zero moment of inertia. It follows that the net force and torque acting on the body must be zero at all times. In other words the body is always in mechanical equilibrium. The equations of equilibrium need to be solved in order to find the tensions in the springs that connect the body to the fluid, and these tensions are needed in order to find the force on the fluid. The formulation of this equilibrium problem is as follows.

In cartesian coordinates that are attached to the body, let

$$\mathbf{Z}_k, \quad k = 1, \ldots, n \tag{1}$$

be the coordinates of the points of the body that are connected to the fluid by stiff springs. We assume that the origin of coordinates within the body has been chosen to be the centroid of these points, and then we have the useful equation

$$\sum_{k=1}^{n} \mathbf{Z}_k = 0. \tag{2}$$

Since the body is rigid, it moves by translation and rotation only. Therefore, the lab-frame position of the point with label $k$ is always of the form

$$\mathbf{X}_0 + R\mathbf{Z}_k, \tag{3}$$

where $\mathbf{X}_0$ is the lab-frame position of the origin of the body coordinates, and where $R$ is a $3 \times 3$ rotation matrix. Note that $\mathbf{X}_0$ and $R$ do not depend on $k$.

Let $\mathbf{X}_k$ be the point in the fluid to which $\mathbf{Z}_k$ is connected by a stiff, zero-rest-length spring, and let the stiffness of this spring be denoted by the constant $K$, which we assume is the same for all of the springs. We allow in the following for external forces to be applied to the $n$ labeled points of the body, with the force $\mathbf{F}_k$ being applied at the point with label $k$.

The equations of equilibrium can then be stated as follows:

$$0 = \sum_{k=1}^{n} \mathbf{F}_k + K\left(\mathbf{X}_k - (\mathbf{X}_0 + R\mathbf{Z}_k)\right), \tag{4}$$

$$0 = \sum_{k=1}^{n} (R\mathbf{Z}_k) \times \left(\mathbf{F}_k + K\left(\mathbf{X}_k - (\mathbf{X}_0 + R\mathbf{Z}_k)\right)\right). \tag{5}$$

Equation (4) states that the total force on the rigid body is zero, and equation (5) states that the total torque on the rigid body is zero. Note that the torque is being measured with respect to the origin of the coordinate system that is attached to the body. This makes no difference, however, since forces that sum to zero have the same torque about any reference point, and equation (4) guarantees that the forces in question do indeed sum to zero.

Equations (4) & (5) can be simplified. In equation (4), the term $R\mathbf{Z}_k$ drops out because $R$ does not depend on $k$ and the $\mathbf{Z}_k$ have zero as their sum, see equation (2). Equation (4) is then easily solved for $\mathbf{X}_0$ with the result

$$\mathbf{X}_0 = \frac{1}{n} \sum_{k=1}^{n} \left(\mathbf{X}_k + \frac{1}{K}\mathbf{F}_k\right). \tag{6}$$

In equation (5), $\mathbf{X}_0$ drops out because it appears in a cross product with a sum that is equal to zero, and of course we also have $R\mathbf{Z}_k \times R\mathbf{Z}_k = 0$. After these simplifications, equation (5) reads as follows:

$$0 = \sum_{k=1}^{n} (R\mathbf{Z}_k) \times \left(\mathbf{F}_k + K\mathbf{X}_k\right). \tag{7}$$

Note that we now have a complete separation of the equilibrium problem into two parts. The unknown translation $\mathbf{X}_0$ has already been determined — it is given by equation (6), which does not involve $R$, and the unknown rotation $R$ remains to be determined by making use of equation (7), in which $\mathbf{X}_0$ does not appear.

We can convert equation (7) into a matrix equation for $R$ in the following way. Take the cross product of both sides of (7) with an arbitrary vector $\mathbf{c}$, and then use the vector identity

$$\begin{aligned}(\mathbf{a} \times \mathbf{b}) \times \mathbf{c} &= -\mathbf{a}(\mathbf{b} \cdot \mathbf{c}) + \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) \\ &= (-\mathbf{a}\mathbf{b}^{\mathrm{T}} + \mathbf{b}\mathbf{a}^{\mathrm{T}})\mathbf{c}. \end{aligned} \tag{8}$$

In this way, since $\mathbf{c}$ is arbitrary, we get the result

$$\begin{aligned} 0 &= \sum_{k=1}^{n} \left( (\mathbf{F}_k + K\mathbf{X}_k)\, \mathbf{Z}_k^T R^T - R\mathbf{Z}_k\, (\mathbf{F}_k + K\mathbf{X}_k)^{\mathrm{T}} \right) \\ &= (RA)^{\mathrm{T}} - RA, \end{aligned} \tag{9}$$

where

$$A = \sum_{k=1}^{n} \mathbf{Z}_k\, (\mathbf{F}_k + K\mathbf{X}_k)^{\mathrm{T}}\,. \tag{10}$$

Besides satisfying equation (9), $R$ should be orthogonal. We can use the singular value decomposition of $A$ to construct such an $R$. Let

$$A = UDV^{\mathrm{T}}, \tag{11}$$

where $U$ and $V$ are orthogonal, and $D$ is diagonal. Then

$$R = VU^{\mathrm{T}} \tag{12}$$

is orthogonal, and

$$RA = VU^{\mathrm{T}}UDV^{\mathrm{T}} = VDV^{\mathrm{T}}. \tag{13}$$

Since this is symmetric, equation (9) is satisfied.

There are some loose ends here that the reader may want to investigate: We have not shown that $R$ is the only orthogonal solution of equation (9), and we have not shown that $R$ is a rotation, i.e., that $\det(R) = +1$. Of course, the latter condition is easily checked once a candidate $R$ has been found.

With the equilibrium equations solved, we have the important result that the total force and torque that were applied to the rigid body are transmitted unchanged to the fluid. For total force, this is an obvious consequence of equation (4), since the total force on the fluid is given by

$$\sum_{k=1}^{n} K((\mathbf{X}_0 + R\mathbf{Z}_k) - \mathbf{X}_k), \tag{14}$$

and this is equal to $\sum_{k=1}^{n} F_k$ by a simple rearrangement of equation (4). The corresponding result for torque is not quite obvious, since the point where the each spring force is applied to the fluid is different from the point at which (minus) that force is applied to the rigid body. The total torque applied to the fluid is given by

$$\sum_{k=1}^{n} (\mathbf{X}_k - \mathbf{X}_0) \times K((\mathbf{X}_0 + R\mathbf{Z}_k) - \mathbf{X}_k). \tag{15}$$

Note, however, that

$$\mathbf{X}_k - \mathbf{X}_0 = (\mathbf{X}_k - (\mathbf{X}_0 + R\mathbf{Z}_k)) + (R\mathbf{Z}_k). \tag{16}$$

When this is substituted into (15), the result can be simplified using $\mathbf{a} \times \mathbf{a} = 0$, and equation (15) becomes

$$\sum_{k=1}^{n} (R\mathbf{Z}_k) \times K((\mathbf{X}_0 + R\mathbf{Z}_k) - \mathbf{X}_k), \tag{17}$$

which is equal to $\sum_{k=1}^{n} (R\mathbf{Z}_k) \times \mathbf{F}_k$ by a simple rearrangement of equation (5). Thus, the change in location of the force application makes no difference, and equation (5) does indeed ensure that the total torque applied to the rigid body is transmitted to the fluid.

It is also of interest to consider the case in which torque is applied directly, instead of being applied through given external forces. It may seem that we have covered this case already, since the applied forces considered above produce a torque

$$\boldsymbol{\tau} = \sum_{k=1}^{n} (R\mathbf{Z}_k) \times \mathbf{F}_k, \tag{18}$$

but this involves a particular dependence of $\boldsymbol{\tau}$ on $R$, and this actually simplifies the determination of $R$ in comparison to the two cases that will be considered below.

The first of these cases is a given lab-frame torque

$$\boldsymbol{\tau} = \boldsymbol{\tau}_0, \tag{19}$$

independent of $R$. This case is applicable if a constant torque is being applied by some mechanism that is fixed in the laboratory frame.

The second possibility [1] is that the torque-generating mechanism is attached to the rigid body itself, and rotates along with that body. This occurs in the case of bacteria such as *E. coli* that have rotary molecular motors embedded in their cell walls. These motors apply torque to flexible flagella that serve as a propulsion mechanism for the bacterium, and of course there is a countertorque applied by these same motors to the bacterium itself. Let the vector sum of all of the countertorques in a frame of reference attached to the body of the bacterium be denoted $\boldsymbol{\tau}_0$, which we assume here is constant. Then the lab-frame torque applied to the bacterium is is given by

$$\boldsymbol{\tau} = R\boldsymbol{\tau}_0. \tag{20}$$

Although this depends on $R$, the manner in which it does so is different from that of equation (18).

Our purpose now is to formulate and solve the equations of equilibrium in the presence of applied torque given by equation (19) or by equation (20). These two cases have a lot in common, and we consider them in parallel. It makes no essential difference to the difficulty of the problem whether the applied forces $\mathbf{F}_k$ are still included or not, so we leave them in place for the sake of generality. The equation for $\mathbf{X}_0$ remains exactly the same as before, and the equilibrium value of $\mathbf{X}_0$ is unaffected by the addition of the the applied torque $\boldsymbol{\tau}_0$ or $R\boldsymbol{\tau}_0$, so we only need to consider the effect on the eqution for $R$.

After putting the equation for $R$ in matrix form in the same manner as before, we get

$$0 = (\boldsymbol{\tau}_0\times) + (RA)^{\mathrm{T}} - RA, \tag{21}$$

or, alternatively,

$$0 = ((R\boldsymbol{\tau}_0)\times) + (RA)^{\mathrm{T}} - RA \tag{22}$$

by applying the torque given by equation (19) or (20), respectively. In the above equations, the 3x3 matrix $A$ has the same definition as before, see equation (10).

The notation $(\mathbf{a}\times)$ that is used here and in the following denotes the 3x3 antisymmetric matrix such that

$$(\mathbf{a}\times)\mathbf{b} = \mathbf{a} \times \mathbf{b} \tag{23}$$

for all $\mathbf{b}$. Note that

$$((R\mathbf{a})\times) = R(\mathbf{a}\times)R^{\mathrm{T}}. \tag{24}$$

[1] For detailed modeling of the case described in this paragraph, see [2]. This paper uses essentially the version of the rigid pIB method described in this Note, but the exposition in the paper is different from how we present it here, and in particular we show here how to improve an approximation that is made in the paper.

This follows from the invariance of the cross product under rotations, that is, $(R\mathbf{a}) \times (R\mathbf{b}) = R(\mathbf{a} \times \mathbf{b})$. This invariance is obvious from the geometric interpretation of the cross project, but it is not so easy to prove algebraically — try it and see! Given the invariance of the cross product, however, it is very straightforward to prove (24).

Because of (24), we can rewrite (22) as

$$\begin{aligned} 0 &= R(\boldsymbol{\tau}_0 \times)R^{\mathrm{T}} + (RA)^{\mathrm{T}} - RA \\ &= R(\boldsymbol{\tau}_0 \times)R^{\mathrm{T}} + A^{\mathrm{T}}R^{\mathrm{T}} - RA, \end{aligned} \tag{25}$$

and then we can multiply by $R^{\mathrm{T}}$ on the left and by $R$ on the right to obtain

$$\begin{aligned} 0 &= (\boldsymbol{\tau}_0 \times) + R^{\mathrm{T}}A^{\mathrm{T}} - AR \\ &= (\boldsymbol{\tau}_0 \times) + (AR)^{\mathrm{T}} - AR \end{aligned} \tag{26}$$

The only difference between (26) and (21) is now that $RA$ has been replaced by $AR$.

We now make use of the singular value decomposition $A = UDV^{\mathrm{T}}$ and we look for $R$ of the form

$$R = R_1 V U^{\mathrm{T}}, \ \text{ so that } RA = R_1 V D V^{\mathrm{T}} \tag{27}$$

in the case of equation (21), and

$$R = V U^{\mathrm{T}} R_1 \ \text{ so that} AR = U D U^{\mathrm{T}} R_1 \tag{28}$$

in the case of equation (26). In these equations, $R_1$ is an unknown orthogonal matrix (not the same matrix in the two cases). After these changes of variables, and a little algebraic manipulation, the two equations become

$$0 = ((V^{\mathrm{T}}\boldsymbol{\tau}_0)\times) + DR_2^{\mathrm{T}} - R_2 D, \ \text{ where } R_2 = V^{\mathrm{T}} R_1 V \tag{29}$$
$$0 = ((U^{\mathrm{T}}\boldsymbol{\tau}_0)\times) + R_2^{\mathrm{T}} D - D R_2, \ \text{ where } R_2 = U^{\mathrm{T}} R_1 U. \tag{30}$$

In each of these equations, $R_2$ is an unknown orthogonal matrix, and everything else is known.

If the applied torque is small in some appropriate dimensionless sense, then we should look for a solution $R_2$ in each case that is close to the identity. An orthognoal matrix close to the identity is (approximately) of the form $I + \Omega$, where

$\Omega$ is small and antisymmetric. If we substitute this form for $R_2$ into (29) or (30), we get

$$0 = ((V^{\mathrm{T}}\boldsymbol{\tau}_0)\times) - D\Omega - \Omega D, \tag{31}$$

$$0 = ((U^{\mathrm{T}}\boldsymbol{\tau}_0)\times) - \Omega D - D\Omega. \tag{32}$$

Note that finally our two equations have reached the same form, although the terms involving the given torque $\boldsymbol{\tau}_0$ are different. If we evaluate the diagonal elements of all terms in either of these equations, we simply get $0 = 0$, but this is not a limitation since $\Omega$ is antisymmetric, and its diagonal elements are therefore known to be equal to zero. From the off-diagonal elements of (31) or (32), we get

$$\Omega_{ij} = \frac{((V^{\mathrm{T}}\boldsymbol{\tau}_0)\times)_{ij}}{D_i + D_j}, \tag{33}$$

$$\Omega_{ij} = \frac{((U^{\mathrm{T}}\boldsymbol{\tau}_0)\times)_{ij}}{D_i + D_j}. \tag{34}$$

for any pair $(i, j)$ such that $i \neq j$. Note that none of the denominators here are zero unless *two* of the singular values $D_i$ of the 3x3 matrix $A$ are equal to zero.

This completes the construction of an approximate solution to either of the two given-torque problems, and a procedure for improving the approximate solution by fixed-point iteration will be discussed below. An important point to note about the approximate solution is that it provides an exact solution to the equations of equilibrium, but at the price of allowing a small deformation of the rigid body. This is because equations (29) or (30) for $R_2$ are solved exactly, but for a matrix $R_2$ that is only approximately orthogonal. Another important remark about the approximation we are making here is that we expect it to improve as the stiffness $K$ of the penalty springs becomes large. In the pIB method, we are really interested in the limit $K \to \infty$, and in that limit applied torques (and also the applied forces) are effectively small. This can be seen formally by dividing all of the equations by $K$ and thinking of $1/K$ as a small parameter. Finally, we remark that existence of an equilibrium solution to the given-torque problems we have been considering is by no means assured, and in fact on physical grounds it seems clear that for any fixed $K$, existence will fail for $\|\boldsymbol{\tau}_0\|$ sufficiently large. This is because there is a limit to how much rotation can increase the lengths of the springs that connect the rigid body to the fluid, so when the applied torque is too large, there may be no orientation of the rigid body in which that torque is balanced. This difficulty disappears, however, if we consider a fixed torque and let $K$ be arbitrarilty large, and that is exactly the situatiton in which our approximation becomes increasingly valid.

The approximation described above can be improved by fixed-point iteration. For this we need the Rodrigues' formula for a rotation in three-dimensional space about a unit vector $\mathbf{a}$ through an angle $\theta$. Such a rotation is described by the 3x3 matrix

$$I + \sin(\theta)(\mathbf{a}\times) + (1 - \cos(\theta))(\mathbf{a}\times)^2. \tag{35}$$

An alternate form that will be more useful for us is

$$I + \frac{\sin(\theta)}{\theta}(\boldsymbol{\omega}\times) + \frac{1 - \cos(\theta)}{\theta^2}(\boldsymbol{\omega}\times)^2, \tag{36}$$

where

$$\theta = \|\boldsymbol{\omega}\| \tag{37}$$

In the form (36) of Rodrigues' formula there is no constraint: the vector $\boldsymbol{\omega}$ can have any (positive) norm, and then $\theta = \|\boldsymbol{\omega}\|$ is to be regarded as a function of $\boldsymbol{\omega}$, and not as an independent variable.

In the following, we use the notation $\Omega$ for the antisymmetric matrix $(\boldsymbol{\omega}\times)$. The consistency of this with our previous use of $\Omega$ will become apparent very soon. We can impose the requirement that $R_2$ should be a rotation by setting $R_2$ in equation (29) or (30) equal to the expression (36). When this is done, we get

$$\begin{aligned} 0 &= ((V^{\mathrm{T}}\boldsymbol{\tau}_0)\times) - \frac{\sin(\theta)}{\theta}(D\Omega + \Omega D) + \frac{1 - \cos(\theta)}{\theta^2}(D\Omega^2 - \Omega^2 D), && (38)\\ 0 &= ((U^{\mathrm{T}}\boldsymbol{\tau}_0)\times) - \frac{\sin(\theta)}{\theta}(\Omega D + D\Omega) + \frac{(1 - \cos(\theta))}{\theta^2}(\Omega^2 D - D\Omega^2). && (39) \end{aligned}$$

In these equations

$$\theta = \|\boldsymbol{\omega}\| = \sqrt{\frac{1}{2}\|\Omega\|^2}, \tag{40}$$

in which the matrix norm in use here is the Frobenius norm.

If the driving torques are small, we expect $\|\Omega\|$ to be small as well, and then $\|\Omega\|^2$ should be even smaller. These considerations suggest the fixed-point iterations

$$\begin{aligned} D\Omega_{m+1} + \Omega_{m+1}D &= \frac{((V^{\mathrm{T}}\boldsymbol{\tau}_0)\times) + \frac{1-\cos\theta_m}{\theta_m^2}(D\Omega_m^2 - \Omega_m^2 D)}{\frac{\sin\theta_m}{\theta_m}}, && (41)\\ \Omega_{m+1}D + D\Omega_{m+1} &= \frac{((U^{\mathrm{T}}\boldsymbol{\tau}_0)\times) + \frac{1-\cos\theta_m}{\theta_m^2}(\Omega_m^2 D - D\Omega_m^2)}{\frac{\sin\theta_m}{\theta_m}}. && (42) \end{aligned}$$

Here $m = 0, 1, 2, \ldots$ is the iteration number, and $\Omega_m$ is antisymmetric for all $m$ by definition. If we start from $\Omega_0 = 0$, then $\Omega_1$ will be precisely the antisymmetric matrix $\Omega$ that was used above to construct the approximate solution $I + \Omega$, see equations (31-32). Each of the equations (41) or (42) is easily solved for the off-diagonal components of $\Omega_{m+1}$ in precisely the same way as the approximate solution was previously found, see equations (33) & (34). If the fixed-point iteration converges, then we have found an orientation of the rigid body that is in equilibrium with the applied forces and torques.

# References


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