Computational Statistical Physics

Part II: Interacting particles and molecular dynamics

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Dynamics of composed particles

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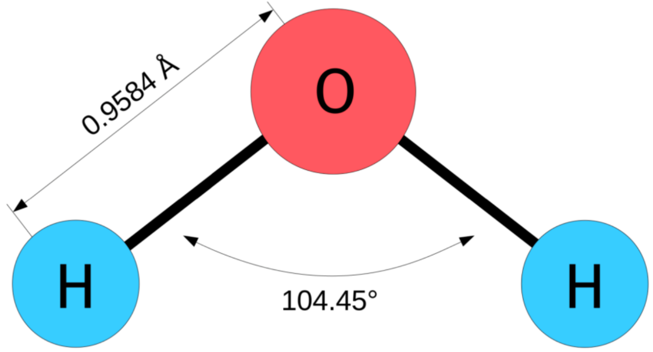

Figure 1: A water molecule as a composed particle system consisting of two hydrogen and one oxygen atom.

Rigid bodies

Rigid bodies

Systems whose n constituents of mass m_i are located at fixed positions x_i are referred to as rigid bodies. The motion of such objects is described by translations of the center of mass and rotations around it. The center of mass is defined as

$$\mathbf{x}_{\mathrm{cm}} = \frac{1}{M} \sum_{i=1}^{n} \mathbf{x}_i m_i \quad \text{with} \quad M = \sum_{i=1}^{n} m_i. \tag{1}$$

Rigid bodies

The equation of motion of the center of mass and the corresponding torque are given by

$$M\ddot{\mathbf{x}}_{\mathrm{cm}} = \sum_{i=1}^{n} \mathbf{f}_i = \mathbf{f}_{\mathrm{cm}} \quad \text{and} \quad \mathbf{M} = \sum_{i=1}^{n} \mathbf{d}_i \wedge \mathbf{f}_i, \tag{2}$$

where $\mathbf{d}_i = \mathbf{x}_i - \mathbf{x}_{\mathrm{cm}}$. In two dimensions, the rotation axis always points in the direction of the normal vector of the plane. Therefore, there exist only three degrees of freedom: two translational and one rotational. In three dimensions, there are six degrees of freedom: three translational and three rotational.

Rigid Bodies 2D

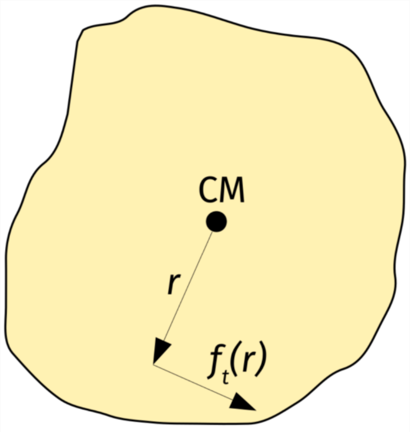

Figure 2: An example of a rigid body in two dimensions. The black dot show the center of mass (CM), and $f_t(r)$ represents the tangential force component.

Rigid Bodies 2D

In two dimensions, the moment of inertia and the torque are given by

$$I = \int \int_A r^2 \rho\left(r\right) \mathrm{dA} \quad \text{and} \quad \mathrm{M} = \int \int_A r f_t\left(r\right) \mathrm{dA}, \tag{3}$$

where f_t is the tangential force. In general, the mass density may be constant or depending on the actual position and not only on the radius r. The equation of motion is given by

$$I\dot{\omega} = \mathrm{M}. \tag{4}$$

Rigid Bodies 2D

We now apply the Verlet algorithm to $\mathbf{x}$ and the rotation angle ϕ to compute the corresponding time evolutions according to

$$\begin{aligned} \phi\left(t+\Delta t\right) &= 2\phi\left(t\right)-\phi\left(t-\Delta t\right)+\Delta t^{2}\frac{\mathrm{M}\left(t\right)}{I}, \\ \mathbf{x}\left(t+\Delta t\right) &= 2\mathbf{x}\left(t\right)-\mathbf{x}\left(t-\Delta t\right)+\Delta t^{2}M^{-1}(t)\sum_{j\in A}f_{j}\left(t\right), \end{aligned} \tag{5}$$

where the total torque is the sum over all the torques acting on the rigid body, i.e.,

$$\mathrm{M}\left(t\right)=\sum_{j\in A}\left[f_{j}^{y}\left(t\right)d_{j}^{x}\left(t\right)-f_{j}^{x}\left(t\right)d_{j}^{y}\left(t\right)\right]. \tag{6}$$

Rigid Bodies 3D

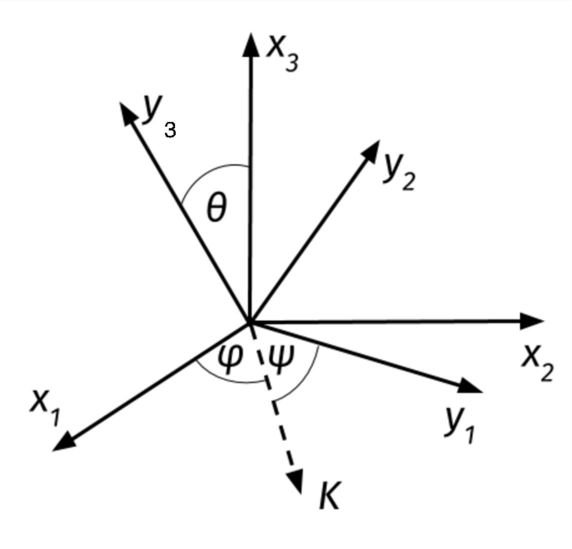

Figure 3: Euler angle parameterization of a rotation matrix.

Rigid Bodies 3D

To describe the motion of rigid bodies in three dimensions, we consider a lab-fixed and a body-fixed coordinate system x and y, respectively. The transformation between both systems is given by

$$\mathbf{x} = R(t)\mathbf{y}, \tag{7}$$

where $R(t) \in \mathrm{SO}(3)$ denotes a rotation matrix[1].

[1] The group $\mathrm{SO}(3)$ is the so-called three dimensional rotation group, or special orthogonal group. All rotation matrices $R \in \mathrm{SO}(3)$ fulfill $R^T R = RR^T = 1$.

Rigid Bodies 3D

Furthermore, we define $\Omega = R^T \dot{R}$ and find with $R^T R = 1$ that

$$R^T \dot{R} + \dot{R}^T R = \Omega + \Omega^T = 0. \tag{8}$$

The latter equation implies that Ω is skew-symmetric and thus of the form

$$\Omega = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \quad \text{and} \quad \Omega \mathbf{y} = \boldsymbol{\omega} \wedge \mathbf{y}, \tag{9}$$

where $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$.

Rigid Bodies 3D

The angular momentum is then given by

$$\mathbf{L} = \sum_{i=1}^{n} m_i \mathbf{x}_i \wedge \dot{\mathbf{x}}_i = \sum_{i=1}^{n} m_i R \mathbf{y}_i \wedge \dot{R} \mathbf{y}_i. \tag{10}$$

Combing Eqs. (10) and (9) yields

$$\mathbf{L} = R \sum_{i=1}^{n} m_i \mathbf{y}_i \wedge (\boldsymbol{\omega} \wedge \mathbf{y}_i) = R \sum_{i=1}^{n} m_i \left[\boldsymbol{\omega} \left(\mathbf{y}_i \cdot \mathbf{y}_i\right) - \mathbf{y}_i \left(\boldsymbol{\omega} \cdot \mathbf{y}_i\right)\right]. \tag{11}$$

Rigid Bodies 3D

The components of the inertia tensor are defined as

$$I_{jk} = \sum_{i=1}^{n} m_i \left[(\mathbf{y}_i \cdot \mathbf{y}_i)\, \delta_{jk} - \mathbf{y}_i^j \mathbf{y}_i^k \right] \tag{12}$$

and thus

$$\mathbf{L} = R\mathbf{S} \quad \text{with} \quad S_j = \sum_{k=1}^{3} I_{jk} \boldsymbol{\omega}_k. \tag{13}$$

where I is the inertia tensor.

Rigid Bodies 3D

Considering a coordinate system whose axes are parallel to the principal axes of inertia of the body, the intertia tensor takes the form

$$I = \begin{pmatrix} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & I_3 \end{pmatrix} \quad \text{and} \quad S_j = I_j \omega_j. \tag{14}$$

Rigid Bodies 3D

With Eq. (13), the equations of motion are determined by

$$\dot{\mathbf{L}} = \dot{R}\mathbf{S} + R\dot{\mathbf{S}} = \widetilde{\mathbf{M}}, \tag{15}$$

where $\widetilde{\mathbf{M}} = R\mathbf{M}$ represents the torque in the lab-fixed coordinate system. By multiplying the latter equation with R^T, we find the *Euler equations* in the principal axes coordinate system, i.e.,

$$\dot{\omega}_1 = \frac{M_1}{I_1} + \left(\frac{I_2 - I_3}{I_1}\right)\omega_2\omega_3, \tag{16}$$

$$\dot{\omega}_2 = \frac{M_2}{I_2} + \left(\frac{I_3 - I_1}{I_2}\right)\omega_3\omega_1, \tag{17}$$

$$\dot{\omega}_3 = \frac{M_3}{I_3} + \left(\frac{I_1 - I_2}{I_3}\right)\omega_1\omega_2. \tag{18}$$

Rigid Bodies 3D

The angular velocities are then integrated according to

$$\omega_1\left(t+\Delta t\right)=\omega_1\left(t\right)+\Delta t\frac{M_1\left(t\right)}{I_1}+\Delta t\left(\frac{I_2-I_3}{I_1}\right)\omega_2\omega_3, \tag{19}$$

$$\omega_2\left(t+\Delta t\right)=\omega_2\left(t\right)+\Delta t\frac{M_2\left(t\right)}{I_2}+\Delta t\left(\frac{I_3-I_1}{I_2}\right)\omega_3\omega_1, \tag{20}$$

$$\omega_3\left(t+\Delta t\right)=\omega_3\left(t\right)+\Delta t\frac{M_3\left(t\right)}{I_3}+\Delta t\left(\frac{I_1-I_2}{I_1}\right)\omega_1\omega_2. \tag{21}$$

Rigid Bodies 3D

From these expressions, we obtain the angular velocity in the laboratory frame

$$\widetilde{\boldsymbol{\omega}}\,(t+\Delta t) = R\boldsymbol{\omega}\,(t+\Delta t)\,. \tag{22}$$

Since the particles are moving all the time, the rotation matrix is not constant. We therefore have to find an efficient way to determine and update R at every step in our simulation. In the following, we therefore discuss Euler angles and quaternions.

Euler angles

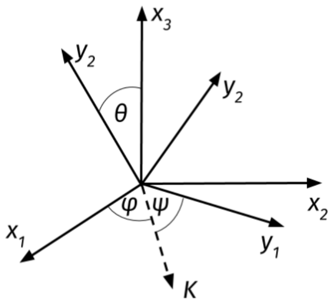

Figure 4: Euler angle parameterization of a rotation matrix.

Euler angles

One possible parameterization of the rotation matrix R is the following:

$$R = R(\phi, \theta, \psi)$$
$$= \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{23}$$

Euler angles

As a consequence of the occurrence of products of multiple trigonometric functions for arbitrary rotations, this parameterization is not well-suited for efficient computations. We have to keep in mind that this operation has to be performed for every particle and every time step, making this approach computationally too expensive. For the computation of angular velocities, derivatives of Eq. (23) have to be considered.

Quaternions

Denis J. Evans, a professor in Canberra, AU, came up with a trick to optimize the computation of rotational velocities [Evans,'77] and replace Euler angles in EoM with Quaternions.

Figure 5: Stone at Brougham Bridge in Dublin where Hamilton came up with the multiplication rule for quaternion. Source: `https://commons.wikimedia.org/`.

Quaternions

Quaternions are a generalization of complex numbers, where four basis vectors span a four-dimensional space. By defining

$$q_0 = \cos\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi+\psi}{2}\right), \tag{24}$$

$$q_1 = \sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\phi-\psi}{2}\right), \tag{25}$$

$$q_2 = \sin\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi-\psi}{2}\right), \tag{26}$$

$$q_3 = \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\phi+\psi}{2}\right), \tag{27}$$

with $0 < q_i < 1$ and $\sum_i q_i = 1$ for $i \in \{1, \ldots, 4\}$, we represent the angles in dependence of a set of quaternions q_i. The Euclidean norm of q equals unity and thus there exist only three independent parameters.

Quaternions

The rotation matrix as defined in Eq. (23) has a quaternion representation, i.e.,

$$R = \begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2\,(q_1 q_2 + q_0 q_3) & 2\,(q_1 q_3 - q_0 q_2) \\ 2\,(q_1 q_2 - q_0 q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2\,(q_2 q_3 + q_0 q_1) \\ 2\,(q_1 q_3 + q_0 q_2) & 2\,(q_2 q_3 + q_0 q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix}. \tag{28}$$

Quaternions

We now found a more efficient way of computing rotations without the necessity of computing lengthy products of sine and cosine functions. This approach much faster than one of Eq. (23). The angular velocities are then computed according to

$$\begin{pmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \begin{pmatrix} 0 \\ \omega_x \\ \omega_y \\ \omega_z \end{pmatrix} \tag{29}$$

Quaternions

Since the world of quaternions and the normal Euclidean space are connected by a diffeomorphism, there is always the possibility of calculating the values of the Euler angles if needed

$$\phi = \arctan\left[\frac{2\left(q_0 q_1 + q_2 q_3\right)}{1 - 2\left(q_1^2 + q_2^2\right)}\right] \tag{30}$$

$$\theta = \arcsin\left[2\left(q_0 q_2 - q_1 q_3\right)\right] \tag{31}$$

$$\psi = \arctan\left[\frac{2\left(q_0 q_3 + q_1 q_2\right)}{1 - 2\left(q_2^2 + q_3^2\right)}\right] \tag{32}$$

Quaternions

There is no need of calculating the Euler angles at each integration step. We now simulate our rigid body dynamics in quaternion representation according to the following strategy:

- Compute the torque $M(t)$ in the body frame.
- Obtain $\omega(t + \Delta t)$ according to Eq. (21) (quaternion representation).
- Update the rotation matrix as defined in Eq. (28) by computing $q(t + \Delta t)$ according to Eq. (29).

Quaternions

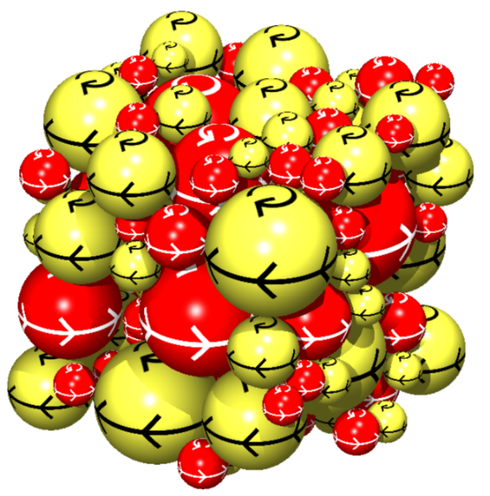

Figure 6: Rotating spheres in a sphere assembly as an example of rigid body dynamics [Stager et al., 2016]