coordinate_systems

Figure 3.3. Definition of the coordinate systems used in formulation of the rigid body equations of motion

We define 3 coordinate systems:

1. - the “global” or a “lab” frame. This is the coordinate’s system that is fixed in the 3D space and doesn’t change in time (no translation or rotation). The coordinates in this system can be regarded as regular Cartesian coordinates, e.g. those commonly provided in the molecular input files (other than the Z-matrix/internal coordinates).
2. – the “moving lab” frame. This system is parallel to the system and has its origin on the center of mass of the moving body/fragment. In this coordinates system the particles of the rigid body can only rotate, since the translational motion is already taken care of by the definition. The center of mass is motionless in this system. The motion of the with respect to describes the translational motion of the RB in the lab frame.
3. – the “body” frame. Similar to the “moving lab” frame, this system is rigidly-connected to the body. Its directions (vectors ) coincide with the principal axes of the inertia tensor. Its origin coincides with the origin of the system. Not only the RB’s center of mass, but also all other points stay motionless in this system. The orientation of the “body” frame with respect to the “moving lab” frame defines the orientation of the rigid body in the global space. The orientation can be most simpler defined by the do products of the vectors defining the systems, , which serves the role of rotational coordinate.

Below, we adopting the Dirac notation for regular vectors, like:

Then,

Or,

Here, , so that

That is:

and

Here, is the position of the center of mass, of the RB. These transformations apply to all points of the RB, , so this can be further clarified:

The center of mass is defined:

Finally, the orientation matrix is defined as the matrix that diagonalizes the inertia tensor written in the “moving lab” frame:

.

Such that is diagonal.

The rotation of the RB by an angle around the unit vector that passes the center of mass is described by the transformation of the orientation matrix:

where is the rotation matrix given by:

,

where is the quaternion that describes the same rotation operation and is a non-redundant representation of the orientation.

In case the rotation of RB is performed with respect to the pivot point, , other than the RB’s center of mass, , the position of center of mass must be transformed according to the same rotation matrix:

The motion of the system takes place in some fixed external (laboratory) coordinate system OI1I2I3 (“lab frame”). In all-atomic MD the coordinates of the atoms, , are expressed in this coordinate system. However, the equations of motion for the rigid body may be expressed and solved much more conveniently in the coordinate system (Oe1e2e3), which is conventionally called body-fixed coordinate system (“body frame”). To construct such system we first separate the translational and rotational motions by considering an intermediate coordinate system O*i1i2i3*, centered on the center of mass of the rigid body and moving with the body. Thus the coordinate of the center of mass is zero in such system. Next, the inertia tensor of the body in O*i1i2i3* system may be computed. Since the inertia tensor is symmetric, it is possible to find such transformation matrix, which diagonalizes the inertia tensor:

 (3.28)

The matrix defines the orientation of the rigid body with respect to the intermediate coordinate system O*i1i2i3* and therefore with respect to the lab frame as well (where the observer is located). Such matrix is usually called an attitude matrix. The body frame may be imagined as a part of the body itself. Thus in this coordinate system the positions of all atoms, constituting the rigid body are time-independent.

In contrast to all-atomic MD the positions of the atoms are indexed by two indices – the index of the atom among other atoms in given rigid body (*i*) and the index of the rigid body, to which the atom belongs (*a*). We also denote the atomic variables by small letters and the rigid-body variables by big letters. Assuming such convention the relation between the atomic coordinates and the rigid-body variables in different coordinate systems is given by the following equations:

 (3.29)

The orientation of the rigid body may be specified in several different ways. Most common choices are the attitude matrix (which is described earlier) or the quaternions. Other alternative choices such as Euler angles, yaw-pitch-roll, Andoer-Deprit variables[200], [201] are less common for molecular dynamics applications. In general, the angular momenta are not conjugate momenta for the orientational variables chosen. Thus the Hamiltonian equations (3.6) are not applicable to the pairs: attitude matrix – angular momentum or quaternion – angular momentum. Instead, the equations of evolution of the orientation variables (3.30, c) and the angular momenta (3.30, d) are derived from the laws of conservation of the angular momenta. The equations for translational variables (3.30, a and b), however, still may be obtained from the Hamilton equations (3.6):

, (3.30)

where defines a skew-symmetric matrix:

 (3.31)

In fact, the skew-symmetric matrices are used here to conveniently represent the vector products, by recalling the identity:

 (3.32)

Integration of the equations of motion for translational variables (position of the central of mass and the translational momentum) is usually performed in the same way as for all-atomic MD, using Verlet-like schemes. The most challenging part of the computations of dynamics of the rigid bodies is related to a solution for rotational variables (e.g. angular momentum and the attitude matrix).