CS273: Algorithms for Structure and Motion in Biology Handout # 1
Stanford University Tuesday, 30 March 2004

Lecture #1:	30 March 2004
Topics:	Rigid Body Transform Geometric and Kinematic Models of Bio Molecules
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1 Rigid Body Transform

Consider a geometric object modeled as a set of points in Euclidean space. By definition, a *rigid body transform* is a mapping from this set to another subset of the Euclidean space, such that the Euclidean distances between points are preserved. Any such mapping can be represented as a composition of one translation and one rotation. We are interested in compact and convenient mathematical description of rigid body transforms.

1.1 2D Case

First consider a two-dimensional Euclidean space, and an object A in it, transformed into the object A' by a rigid body transform (Figure 1). Suppose that points are described by standard Cartesian coordinate pairs in the coordinate system xOy. Then obviously, any transform which takes A into A' also takes xOy (treated as a 2D object) into $x'Oy'$, such that the representation of A' in $x'Oy'$ is the same as the one of A in xOy. For example, in Figure 1, both A and xOy are translated along the vector $\boldsymbol{t} = [\ t_x \quad t_y\ ]^T$ in the original coordinate system, and then rotated by the angle θ. Therefore, $(\boldsymbol{t}, \theta)$ is one possible description of the transform. In particular, the position of O' in the original coordinate system xOy is given by $\boldsymbol{t}$ (this is the translation part of the transform), whereas the unit vectors $\boldsymbol{i} = [\ i_1 \quad i_2\ ]^T$ and $\boldsymbol{j} = [\ j_1 \quad j_2\ ]^T$ of $x'Oy'$ are the columns of the 2D *rotation matrix*

$$R = \begin{bmatrix} i_1 & j_1 \\ i_2 & j_2 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.$$

R describes the rotation part of the transform, i.e. the rotation of xOy around the origin. This represents the transform of the object as a whole. To relate an arbitrary point $A(x, y)$ to its image $A'(x', y')$, recall that A' is represented in $x'Oy'$ by the same coordinates as A in $x'Oy'$, and use elementary vector algebra

$$\begin{bmatrix} x' \\ y' \end{bmatrix} \; = \; \boldsymbol{t} + x\boldsymbol{i} + y\boldsymbol{j} \; = \; \boldsymbol{t} + R \begin{bmatrix} x \\ y \end{bmatrix}$$

The above relation can be compactly expressed if we introduce *homogeneous coordinates* [1], which (for our current purposes) amounts to adding a third coordinate equal to 1.

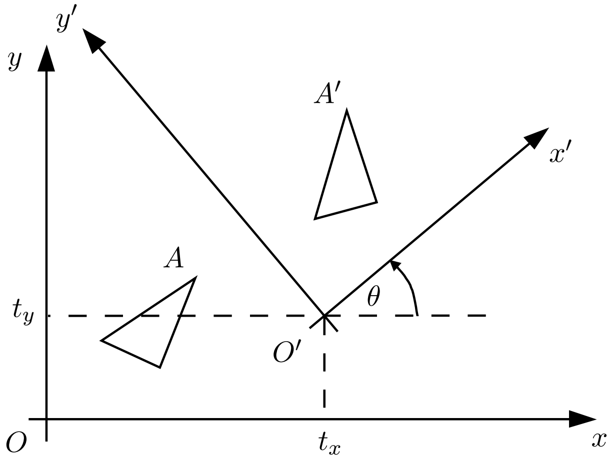

Figure 1: Rigid body transform of a 2D coordinate system

Now, the translation and rotation components can be encoded in the same matrix

$$\begin{bmatrix} x' \\ y' \\ 1 \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & t_x \\ \sin\theta & \cos\theta & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} i_1 & j_1 & t_x \\ i_2 & j_2 & t_y \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 1 \end{bmatrix}. \tag{1}$$

With this representation it is easy to compose transforms. If M_1 and M_2 represent T_1 and T_2, respectively, then $T(\cdot) = T_2(T_1(\cdot))$ is represented by $M = M_2 M_1$. Note that M has the same format as M_1 and M_2, meaning that the translation vector and rotation angle of the composite mapping can be directly read from it.

Rotation matrix has four entries, but only one number (θ) is sufficient to uniquely specify a rotation. That means that representing rotations by rotation matrices is somewhat redundant. Indeed, the four entries are not independent, because they must satisfy the orthonormality constraints

$$i_1^2 + i_2^2 = 1 \qquad i_1 j_1 + i_2 j_2 = 0 \qquad \begin{vmatrix} i_1 & j_1 \\ i_2 & j_2 \end{vmatrix} = +1$$

which remove the three additional degrees of freedom. The above conditions can be also expressed as $R^T R = I$, $\det R = +1$, where I is the 2×2 identity matrix.

1.2 3D Case

In three-dimensional space, rigid body transforms are composed of translations along three-dimensional vectors and rotations around coordinate axes. Compositions of transforms are harder to visualize, and determining the translation and rotation components of composite mappings is not easy to do using only geometric and trigonometric relations. Fortunately, the algebraic formalism developed in two dimensions completely carries over to this case. In particular, when points are represented with homogeneous coordinates, a three-dimensional transform is encoded into a 4×4 matrix

$$\begin{bmatrix} i_1 & j_1 & k_1 & t_x \\ i_2 & j_2 & k_2 & t_y \\ i_3 & j_3 & k_3 & t_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where $\boldsymbol{i} = [\ i_1 \quad i_2 \quad i_3\ ]^T$, $\boldsymbol{j} = [\ j_1 \quad j_2 \quad j_3\ ]^T$ and $\boldsymbol{k} = [\ k_1 \quad k_2 \quad k_3\ ]^T$ are the unit vectors of the transformed coordinate system, while $\boldsymbol{t} = [\ t_x \quad t_y \quad t_z\ ]^T$ is the position of its origin with respect to the original coordinate system. The sub-matrix which defines the rotation part of the transform

$$R = \begin{bmatrix} i_1 & j_1 & k_1 \\ i_2 & j_2 & k_2 \\ i_3 & j_3 & k_3 \end{bmatrix}$$

must again be orthonormal

$$R^T R = I \qquad \det R = +1 \tag{2}$$

where I is the 3×3 identity matrix. For example, the rotation around y-axis by θ is represented by

$$R = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}.$$

Mapping of individual points is a generalization of (1)

$$\begin{bmatrix} x' \\ y' \\ z' \\ 1 \end{bmatrix} = \begin{bmatrix} i_1 & j_1 & k_1 & t_x \\ i_2 & j_2 & k_2 & t_y \\ i_3 & j_3 & k_3 & t_z \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}.$$

The composition of transforms again amounts to multiplying matrices.

Due to the constraints (2) that the rotation matrix satisfies, its nine entries are redundant representation of rotation. There are various other representations with less redundancy. We will consider Euler angles and quaternions.

1.3 Euler Angles

Consider a Cartesian coordinate system S and its rotated version S'. We can make S coincide with S' by performing three consecutive canonical rotations on it. Starting from $S = S_1$, we first rotate around z-axis by ϕ obtaining S_2, then around y-axis by θ obtaining S_3, and finally around z-axis by ψ, obtaining $S_4 = S'$ (Figure 2). Obviously, any rotation between S and S' can be decomposed in this way, with ϕ, θ and ψ appropriately chosen,

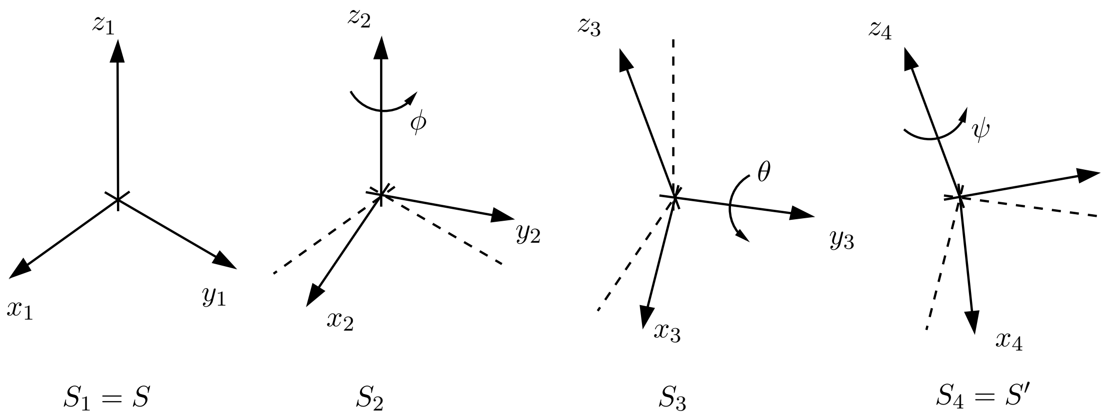

Figure 2: Euler angles

so the triple of *Euler angles* (ϕ, θ, ψ) can be used to uniquely define the rotation. Note that this is a three number description, clearly more compact than a rotation matrix. Given the Euler angles, it is easy to go to the rotation matrix representation: one only needs to multiply the rotation matrices for the three elementary rotations

$$\begin{bmatrix} i_1 & j_1 & k_1 \\ i_2 & j_2 & k_2 \\ i_3 & j_3 & k_3 \end{bmatrix} = \begin{bmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

However, given the rotation matrix on the right hand side, the Euler angles cannot always be determined uniquely, i.e. the corresponding trigonometric equations has *uncountably* infinite set of solutions for (ϕ, θ, ψ). For example, if our rotation leaves the z-axis unchanged $(\theta = 0)$, then any (ϕ, ψ) combination such that ϕ and ψ add up to the same number represents the same rotation. It turns out that this problem cannot be avoided even if we choose any other set of canonical angles to represent rotations by. So, the mapping from the set of Euler angle triples (no matter how we choose the angles) to the set of 3D rotations is inherently "many to one".

1.4 Quaternions

Another way to compactly represent a rotation is by identifying it with a point on a three-dimensional unit sphere embedded into the four-dimensional Euclidean space. In other words, a rotation is represented by a four-tuple of real numbers whose Euclidean norm is one. This 4D space, equipped with appropriate operations on four-tuples (to be defined below) is referred to as the space of *quaternions*. Specifically, quaternions with unit Euclidean norm are called *unit quaternions*.

In particular, rotations by θ around the axis parallel to $\boldsymbol{r} = (r_1, r_2, r_3)$, $\|\boldsymbol{r}\| = 1$, is represented by the unit quaternion

$$\boldsymbol{R}(\boldsymbol{r}, \theta) = \cos(\theta/2) + \boldsymbol{r}\sin(\theta/2) = (\cos(\theta/2), r_1 \sin(\theta/2), r_2 \sin(\theta/2), r_3 \sin(\theta/2))$$

Notice that if two rotations about the same axis have angles which differ by 2π, it is natural to consider them identical. However, the corresponding quaternions will be different, more precisely antipodal on the 3D unit sphere. In other words, the correspondence between the set of unit quaternions and the set of 3D rotations is two to one. Therefore, for the purposes of representing rotations, we consider the space of unit quaternions with modified connectivity – antipodal points on the unit sphere are identified.

It is convenient to view a quaternion $\boldsymbol{P}$ as the "sum" of the "scalar" part p_0 (the first component of the 4-tuple), and the remaining three-dimensional "vector" part $\boldsymbol{p}$. This way, the operations on quaternions can be defined more easily, by referring to the standard vector operations in 3D space. For any two (not necessarily unit) quaternions $\boldsymbol{P} = p_0 + \boldsymbol{p}$ and $\boldsymbol{Q} = q_0 + \boldsymbol{q}$ we define the *product* $\boldsymbol{R} = r_0 + \boldsymbol{r}$ by

$$r_0 = p_0 q_0 - \boldsymbol{p} \cdot \boldsymbol{q} \qquad \boldsymbol{r} = p_0 \boldsymbol{q} + q_0 \boldsymbol{p} + \boldsymbol{p} \times \boldsymbol{q}$$

where "$\cdot$" and "$\times$" respectively denote dot product and cross product of 3D vectors. The *conjugate* of $\boldsymbol{P}$ is obtained by changing the sign of the vector part

$$\boldsymbol{P}^* = p_0 - \boldsymbol{P}$$

A point (x, y, z) in 3D space is represented by a vector $\boldsymbol{x} = [\; x \quad y \quad z \;]^T$, i.e. by a quaternion with scalar part equal to zero, $\boldsymbol{X} = 0 + \boldsymbol{x}$.

The coordinate vector $\boldsymbol{x'}$ of the point obtained from $\boldsymbol{x}$ after translation $\boldsymbol{t}$ and rotation $(\boldsymbol{n}, \theta)$, is given by

$$0 + \boldsymbol{x'} = \boldsymbol{R}(\boldsymbol{n}, \theta)\ (0 + \boldsymbol{x})\ \boldsymbol{R}^*(\boldsymbol{n}, \theta) + (0 + \boldsymbol{t}) \tag{3}$$

The composition of rotations $(\boldsymbol{n_1}, \theta_1)$ and $(\boldsymbol{n_2}, \theta_2)$ corresponds to the product of the quaternions $\boldsymbol{R}(\boldsymbol{n_2}, \theta_2)\boldsymbol{R}(\boldsymbol{n_1}, \theta_1)$.

Redundancy of the quaternion representation is small. It requires four values, and only three are sufficient to define a rotation in 3D space. One degree of freedom is removed by the unit norm constraint. While Euler angle representation is more compact, it is harder to use it in practice, because there is no direct way to perform computations on coordinate vectors. Quaternion representation, however, allows direct mapping of Cartesian coordinates, using the operations in the space of unit quaternions, as in (3).

More details about quaternions can be found in [1].

2 Geometric Models of Bio Molecules

We shall explain two ways to model the shape of biological molecules: the hard sphere model and the solvent accessible model.

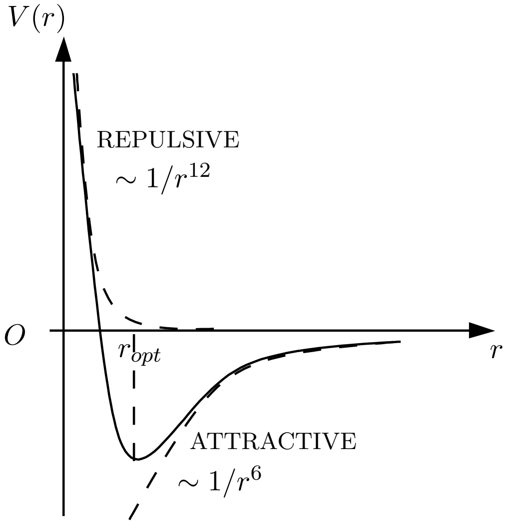

Figure 3: Van der Waals potential energy

In the *hard sphere* model, each atom of the molecule is modeled as a sphere whose radius depends on the atom (more precisely, the chemical element). The radius of the sphere is taken to be equal to the *Van der Waals radius* of the corresponding element. Van der Waals interactions (forces) between atoms are a consequence of induced polarization, i.e. formation of electric dipoles in atoms when they are close to each other. These forces are weak except over short ranges. Like many other interactions in nature, they can be represented by a potential energy function (Figure 3), which in this case depends only on the distance r between atom centers. One commonly used model of this dependence is *12-6 Lennard-Jones Potential*

$$V_{12-6}(r) = 4\epsilon_{XY}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

where ϵ_{XY} and σ are empirical parameters. This kind of potential energy is a combination of attractive interactions, proportional to $1/r^6$ and dominant for $r > r_{opt}$, and repulsive interactions, proportional to $1/r^{12}$ and dominant for $r < r_{opt}$. The state of stable equilibrium, when attractive and repulsive forces are balanced, corresponds to $r = r_{opt}$. Van der Waals radius, as a property of a chemical element, is defined to be one half of the equilibrium distance between two interacting atoms of that chemical element. Table 1 shows Van der Waals radius values for some elements.

Element	H	C	N	O	F	P	S	Cl
Van der Waals radius (Å)	1.2	1.7	1.5	1.4	1.35	1.9	1.85	1.8

Table 1: Van der Waals radii of certain chemical elements

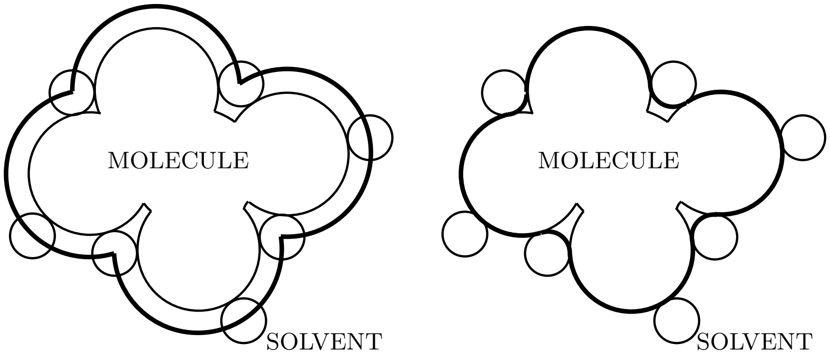

Figure 4: Solvent accessible models: accessible surface model (left) and molecular surface model (right)

Solvent accessible model [2] takes into account the surface of the molecule which can come into contact with a molecules of the solvent (e.g. water). Solvent molecule (*probe*) is represented by a single sphere, even though it usually consists of more than one atom. Bio molecule under consideration is typically a polymer chain, much larger in size than the surrounding solvent molecules. Two examples of this approach are shown in Figure 4. *Accessible surface model* considers the closed surface traced by a solvent molecule as it goes through all possible positions in which the two molecules are in surface contact. *Molecular surface model* is similar. It defines a surface composed of many surface patches, some of which are defined by the surface of the macromolecule, while others come from the surface of the solvent molecule in positions where the surface contact is established along the closed curve, not only at one point. What is common to these models is some degree of "smoothing" of the hard sphere representation of the surface. Obviously, the level of details grows as the radius of the sphere which models the solvent molecule becomes smaller.

3 Kinematic Models of Bio Molecules

Kinematics studies motion of objects in space, independent of the forces that cause it. The main goal is to analytically describe the positions of objects and how they evolve in time. In case of bio molecules, the objects of interest are individual atoms. Their positions are typically described by atomistic model or linkage model.

In *atomistic model*, configuration of atoms in the molecule at any point in time is described simply by listing the coordinates of their centers, as points in 3D space, with respect to some external coordinate system. This description requires three values per atom, but since we do not distinguish between rigid body transforms of the molecule as a whole, the six degrees of freedom (three translational and three rotational) should be subtracted from the total number.

In *linkage model*, position of each atom is defined with respect to certain other atoms,

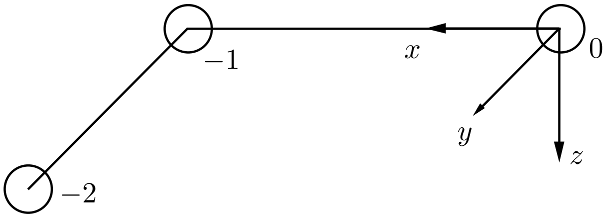

Figure 5: Local coordinate frame

i.e. using a local coordinate system. Each local coordinate system is used for only a small group of atoms.

Linkage model usually makes use of the fact that the molecules under consideration are long chain-like polymers (proteins, nucleic acids), and considers atoms inside local frames of reference, defined by their predecessors in the chain. The main quantities that define positions within such frames are bond lengths, bond angles and torsion angles (dihedral angles).

First consider a hypothetical molecule whose atoms are arranged in a simple chain. We build its linkage model as follows. Since we do not distinguish between the rigid body transforms of the whole molecule, we can use the first three atoms (usually denoted by -1, -2, 0) in the chain to define the initial coordinate frame, as shown in Figure 5. Within this frame we consider the position of the fourth atom in the chain (atom 1). In principle, any type of coordinate axes (Cartesian, spherical etc), can be built using the three atoms. However, it is customary to use the representation shown in Figure 6. First translate atom 0 in the direction of atom -1 by the the distance equal to the *length of the bond* between atoms 0 and 1. Then rotate the image, in the plane defined by the atoms -2, -1, 0, by the *angle between the bonds* connecting atom -1 to atom 0 and atom 0 to atom 1. Finally, do another rotation around the axis passing through atoms -1 and 0, to bring the image to the position of atom 1. The angle of the last rotation is called *rotation angle* or *torsion angle.* In summary, position of the atom 1 within its local frame of reference defined by the atoms -2, -1, 0 is represented by the bond length d, bond angle θ and torsion angle ϕ. The same process continues along the chain, namely the position of atom i is expressed within the coordinate system defined by the atoms $i-3$, $i-2$ and $i-1$, with origin in the position of atom $i-1$. Composition of the three transformations (translation and two rotations) actually takes the local frame of atom $i-1$ to the next local frame of atom i. The corresponding transformation matrix is

$$T_i = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\phi & \sin\phi & 0 \\ 0 & -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta & 0 & 0 \\ \sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & d \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

As a base case, T_0 is defined to be the mapping from the global ("world") coordinate

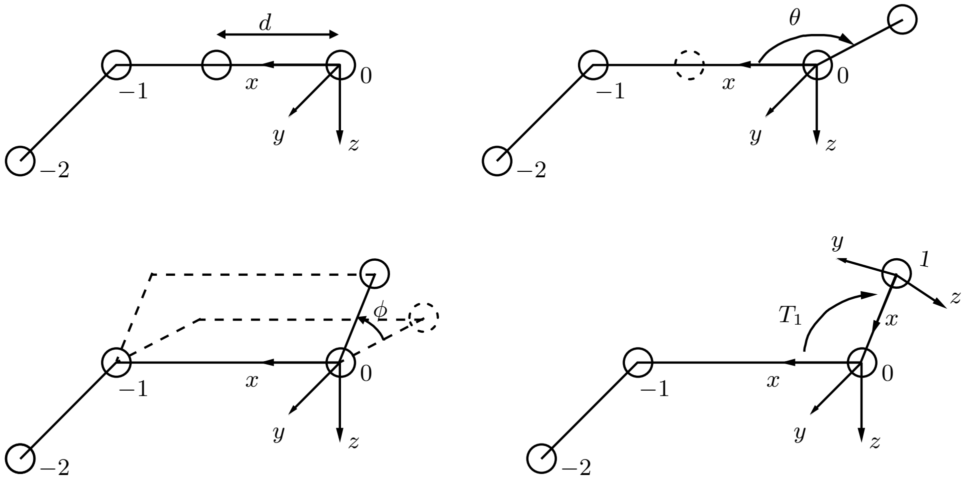

Figure 6: Local coordinates of an atom: bond length d (upper left), bond angle θ (upper right), torsion angle ϕ (lower left), transform between consecutive local frames (lower right)

system to the local coordinate system of atom 0. As noted above, this is the identity map if we don't care about rigid motions of the whole molecule.

When molecule is a simple chain, each atom is placed inside different local frame, except atoms -2, -1, 0, for which we need to specify only lengths of the bonds between atom pairs -2, -1 and -1, 0, as well as the angle between these two bonds. Everything else is implicitly defined by identifying the local frame of atom 0 with the global system. Only 3 (instead of 9) coordinates are used for the three initial atoms, which corresponds to the removal of six degrees of freedom corresponding to rigid body transforms, as mentioned above.

For $i < k$, the frame of atom i is mapped to the frame of atom k by transform $T_{i \to k} = T_{i+1} T_{i+2} \cdots T_k$. If the position of atom j, $i < j < k$ changes, four transformation matrices (T_j, T_{j+1}, T_{j+2}, T_{j+3}) need to be updated, in the worst case.

If the atoms do not form a chain, it might be possible to find a (connected) group of three atoms which, when collapsed into a single atom, becomes a root of a tree structure. In other words, these are the cases when the bonds do not form cycles, except within the three-atom group serving as the root. Then the local frame for each atom is defined by the three atoms closest to it on the (unique) path to the root. Initial frame is defined by the three atoms inside the root. The tree condition is satisfied by many biological molecules, or at least approximately satisfied, because many cyclic components (e.g. aromatic rings in amino acids) can be treated as rigid, essentially as single atoms.

Both atomistic and linkage models have advantages and drawbacks. Atomistic model emphasizes properties of the molecules such as atomic interactions, which depend on relative positions of arbitrary atoms, and not on the chain structure. In linkage models, computing distances requires going through potentially long series of matrix multiplications along the chain. For the same reason, linkage models are less numerically robust, since numerical errors accumulate. On the other hand, imposing constraints on bond angles and bond lengths is easily accomplished in linkage models, by using the corresponding atom coordinates. In atomistic representation, bonds are not modeled directly, so these constraints would have to be included at the expense of adding more parameters to the model.

In most practical cases, variations in bond lengths and bond angles are much smaller than variations in torsion angles. This gives rise to a widely used simplified linkage model. Bond lengths and bond angles are assumed to be fixed, and the only remaining degrees of freedom are torsion angles. This representation requires only one number per atom.

References

[1] CS348A: Computer Graphics – Geometric Modeling, course reader

[2] T. E. Creighton, “Proteins: Structures and Molecular Properties”, *W. H. Freeman and Company*, pages 227-232, second edition, 1993.