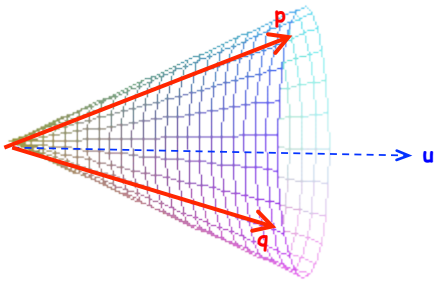
Mesoscale modeling

In the past few decades great strides have been made in chemistry at the nanoscale, where the atomic granularity of matter and the exact positions of individual atoms are key determinants of structure and dynamics. Less attention, however, has been paid to the mesoscale--it is at this scale, in the range extending from large molecules (10 nm) through viruses to eukaryotic cells (10 microns), where interesting ensemble effects and the functionality that is critical to macroscopic phenomenon begins to manifest itself and cannot be described by laws on the scale of atoms and molecules alone. Thus, mesoscale systems bridge the molecular and the macroscopic.

Mesoscale Chemistry, A Workshop Summary Chemical Sciences Roundtable; Board on Chemical Sciences and Technology; Division on Earth and Life Studies; National Research Council.Washington (DC): National Academies Press; 2015 Aug 6.

General rotation matrix

Derivation of general rotation matrix **R**(φ, **u**)
(operation that rotates vector **p** about axis **u** by angle φ to new position **q**)



Derivation of general rotation matrix **R**(φ, **u**)
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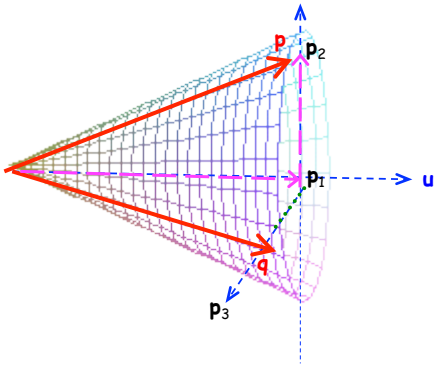


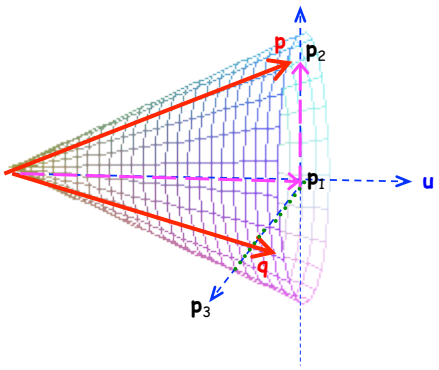
$\mathbf{p}_1 = (\mathbf{p} \cdot \mathbf{u})\mathbf{u}$

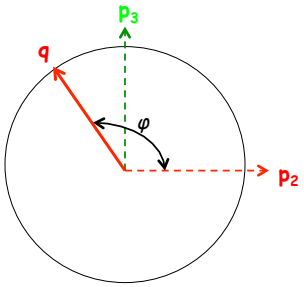
$\mathbf{p}_2 = \mathbf{p} - \mathbf{p}_1$

$\mathbf{p}_3 = \mathbf{p}_1 \times \mathbf{p}_2$

Position **q** can be expressed as a sum of the vectorial components of **p**.

$$\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2 \cos\varphi + \mathbf{p}_3 \sin\varphi = \mathbf{R}(\varphi,\mathbf{u})\,\mathbf{p}$$





The vectorial components of **p** can also be expressed in terms of the elements of **p** = (p_x, p_y, p_z) and **u** = (u_1, u_2 u_3).

$$\mathbf{p}_1 = \left(\mathbf{p}\cdot\mathbf{u}\right)\mathbf{u}$$

$$\mathbf{p}_1 = \left(p_x u_1 + p_y u_2 + p_z u_3\right)\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\mathbf{p}_1 = \begin{bmatrix} p_x u_1^2 + p_y u_1 u_2 + p_y u_1 u_3 \\ p_x u_1 u_2 + p_y u_2^2 + p_z u_2 u_3 \\ p_x u_1 u_3 + p_z u_2 u_3 + p_z u_3^2 \end{bmatrix}$$

$$\mathbf{p}_1 = \begin{bmatrix} u_1^2 & u_1 u_2 & u_1 u_3 \\ u_1 u_2 & u_2^2 & u_2 u_3 \\ u_1 u_3 & u_2 u_3 & u_3^2 \end{bmatrix}\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

The vectorial components of **p** can also be expressed in terms of the elements of **p** = (p_x, p_y, p_z) and **u** = (u_1, u_2 u_3).

$$\mathbf{p}_2 = \mathbf{p} - \mathbf{p}_1$$

$$\mathbf{p}_2 = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} - \begin{bmatrix} u_1^2 & u_1 u_2 & u_1 u_3 \\ u_1 u_2 & u_2^2 & u_2 u_3 \\ u_1 u_3 & u_2 u_3 & u_3^2 \end{bmatrix}\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

$$\mathbf{p}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} - \begin{bmatrix} u_1^2 & u_1 u_2 & u_1 u_3 \\ u_1 u_2 & u_2^2 & u_2 u_3 \\ u_1 u_3 & u_2 u_3 & u_3^2 \end{bmatrix}\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

$$\mathbf{p}_2 = \begin{bmatrix} 1-u_1^2 & -u_1 u_2 & -u_1 u_3 \\ -u_1 u_2 & 1-u_2^2 & -u_2 u_3 \\ -u_1 u_3 & -u_2 u_3 & 1-u_3^2 \end{bmatrix}\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

The vectorial components of **p** can also be expressed in terms of the elements of **p** = (p_x, p_y, p_z) and **u** = (u_1, u_2 u_3).

$$\mathbf{p}_3 = \mathbf{p}_1 \times \mathbf{p}_2$$

$$\mathbf{p}_3 = \begin{bmatrix} u_1^2 & u_1u_2 & u_1u_3 \\ u_1u_2 & u_2^2 & u_2u_3 \\ u_1u_3 & u_2u_3 & u_3^2 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} \times \begin{bmatrix} 1-u_1^2 & -u_1u_2 & -u_1u_3 \\ -u_1u_2 & 1-u_2^2 & -u_2u_3 \\ -u_1u_3 & -u_2u_3 & 1-u_3^2 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

…

…

$$\mathbf{p}_3 = \begin{bmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

General rotation matrix **R**(φ, **u**)
(used to effect the rotation of a vector **p** about an arbitrary unit vector **u** through an angle of magnitude φ to new position **q**)

$$\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2 \cos\varphi + \mathbf{p}_3 \sin\varphi = \mathbf{R}\left(\varphi, \mathbf{u}\right)\mathbf{p}$$

$$\mathbf{p}_1 = \begin{bmatrix} u_1^2 & u_1u_2 & u_1u_3 \\ u_1u_2 & u_2^2 & u_2u_3 \\ u_1u_3 & u_2u_3 & u_3^2 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

$$\mathbf{p}_2 = \begin{bmatrix} 1-u_1^2 & -u_1u_2 & -u_1u_3 \\ -u_1u_2 & 1-u_2^2 & -u_2u_3 \\ -u_1u_3 & -u_2u_3 & 1-u_3^2 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

$$\mathbf{p}_3 = \begin{bmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

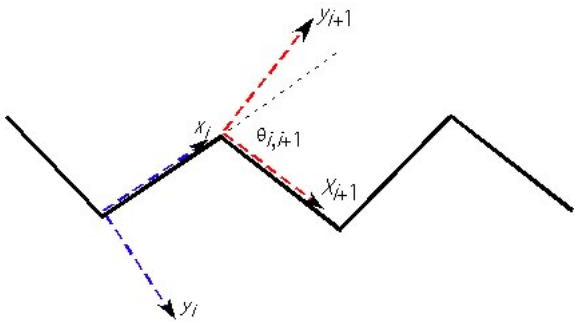
General rotation matrix $\mathbf{R}(\varphi, \mathbf{u})$
(used to effect the rotation of a vector $\mathbf{p}$ about an arbitrary unit vector $\mathbf{u}$ through an angle of magnitude φ to new position $\mathbf{q}$)

$$\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2 \cos\varphi + \mathbf{p}_3 \sin\varphi = \mathbf{R}\left(\varphi, \mathbf{u}\right)\mathbf{p}$$

$$\mathbf{R}\left(\varphi, \mathbf{u}\right) = \begin{bmatrix} \cos\varphi + \left(1-\cos\varphi\right)u_1^2 & u_1u_2\left(1-\cos\varphi\right) - u_3\sin\varphi & u_1u_3\left(1-\cos\varphi\right) + u_2\sin\varphi \\ u_1u_2\left(1-\cos\varphi\right) + u_3\sin\varphi & \cos\varphi + \left(1-\cos\varphi\right)u_2^2 & u_2u_3\left(1-\cos\varphi\right) - u_1\sin\varphi \\ u_1u_3\left(1-\cos\varphi\right) - u_2\sin\varphi & u_2u_3\left(1-\cos\varphi\right) + u_1\sin\varphi & \cos\varphi + \left(1-\cos\varphi\right)u_3^2 \end{bmatrix}$$

Chemical variables in coordinate transformations

Consider a system of coordinate frames embedded on successive chemical bonds
(*x*-axis lies along bond; *y*-axis lies in plane of bond and its predecessor)



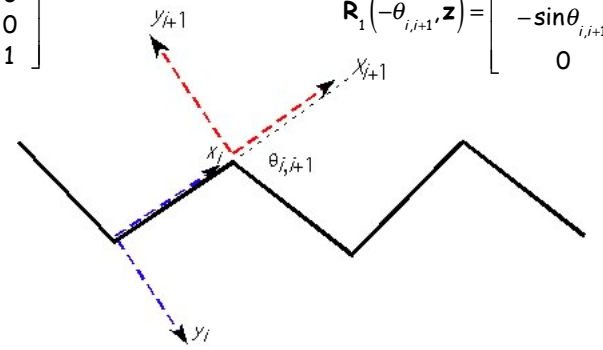
Special case of all-*trans* chain backbone

$\Theta_{i,i+1}$ is the supplement to the valence angle between the bonds in frames *i* and *i*+1

Transformation of frame *i*+1 to frame *i*
(Step 1: rotate frame *i* +1 by $-\theta$ about the *z*-axis of bond *i*+1)

$$\mathbf{u} \rightarrow \mathbf{z} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\mathbf{R}_1\left(-\theta_{i,i+1}, \mathbf{z}\right) = \begin{bmatrix} \cos\theta_{i,i+1} & \sin\theta_{i,i+1} & 0 \\ -\sin\theta_{i,i+1} & \cos\theta_{i,i+1} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

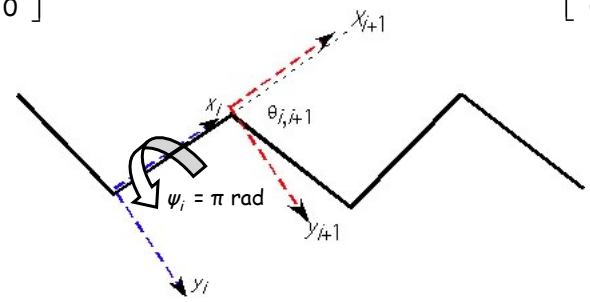


Special case of all-*trans* chain backbone

$\Theta_{i,i+1}$ is the supplement to the valence angle between the bonds in frames *i* and *i*+1

Transformation of frame i+1 to frame i
(Step 2: rotate frame i +1 by π radians about the x-axis of bond i)

$$\mathbf{u} \rightarrow \mathbf{x} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad \mathbf{R}_2(\pi, \mathbf{x}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Special case of all-*trans* chain backbone

Coordinates of bond i+1 in frame i
(premultiply coordinates in frame i+1 by $\mathbf{R}_2(\pi,\mathbf{x})\,\mathbf{R}_1(-\theta,\mathbf{z})$)

$$\mathbf{l}'_{i:i+1} = \mathbf{R}_2(\pi, \mathbf{x})\mathbf{R}_1(-\theta_{i,i+1}, \mathbf{z})\mathbf{l}_{i:i+1}$$

$$\mathbf{l}'_{i,i+1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos\theta_{i,i+1} & \sin\theta_{i,i+1} & 0 \\ -\sin\theta_{i,i+1} & \cos\theta_{i,i+1} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} l \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} l\cos\theta_{i,i+1} \\ l\sin\theta_{i,i+1} \\ 0 \end{bmatrix}$$

Here l is the length of the chemical bond in frame i+1, $\theta_{i,i+1}$ is the supplement to the valence angle between the bonds in frames i and i+1, and π is a rotation of π radians (180°) about the x-axis of frame i.

Special case of all-*trans* chain backbone

Coordinates of bond i+1 in frame i
(premultiply coordinates in frame i by $\mathbf{R}(\psi_i,\mathbf{x}_i)\,\mathbf{R}(-\theta_{i,i+1},\mathbf{z}_{i+1})$)

$$\mathbf{l}'_{i,i+1} = \mathbf{R}_2\left(\psi_i,\mathbf{x}\right)\mathbf{R}_1\left(-\theta_{i,i+1},\mathbf{z}\right)\mathbf{l}_{i,i+1}$$

$$\mathbf{l}'_{i,i+1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\psi_i & -\sin\psi_i \\ 0 & \sin\psi_i & \cos\psi_i \end{bmatrix}\begin{bmatrix} \cos\theta_{i,i+1} & \sin\theta_{i,i+1} & 0 \\ -\sin\theta_{i,i+1} & \cos\theta_{i,i+1} & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} l \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} l\cos\theta_{i,i+1} \\ l\sin\theta_{i,i+1}\cos\psi_i \\ -l\sin\theta_{i,i+1}\sin\psi_i \end{bmatrix}$$

Again l is the length of the chemical bond in frame i+1 and $\theta_{i,i+1}$ the supplement to the valence angle between the bonds in frames i and i+1. The quantity ψ_i is the rotation angle about bond i (relative to a value 0° in the cis orientation).

General case, where ψ_i is the torsion angle about bond i

Polymer chain generation in terms of chemical variables

Chain generation from internal chemical/virtual parameters
($\mathbf{r}_{1:N}$: coordinates of atom N+1 in coordinate frame along bond vector $\mathbf{v}_{12}$)

$$\mathbf{r}_{1:N} = \mathbf{v}_{1:2} + \mathbf{T}_{1:2:3}\mathbf{v}_{2:3} + \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{v}_{3:4} + \cdots + \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\cdots\mathbf{T}_{N-1:N:N+1}\mathbf{v}_{N:N+1}$$

- Each bond vector $\mathbf{v}_{n:n+1}$ is expressed in a local coordinate frame that originates at atom n.
- Premultiplication of vector $\mathbf{v}_{n:n+1}$ by transformation matrix $\mathbf{T}_{n-1:n:n+1}$ converts $\mathbf{v}_{n:n+1}$ to the frame of the preceding bond vector $\mathbf{v}_{n-1:n}$.
- Serial multiplication of each bond vector by the appropriate number of successive transformation matrices makes it possible to express the chain in a common coordinate frame (here along the first bond).

Transformation of coordinates of bond n:n+1 to frame of bond n–1:n
(premultiply coordinates of bond vector $\mathbf{v}_{n:n+1}$ connecting atoms n and n+1 by $\mathbf{R}_2(\psi,\mathbf{x}_{n-1})\,\mathbf{R}_1(-\theta,\mathbf{z}_n)$ and add transformed vector to the coordinates of the vector $\mathbf{v}_{n-1:n}$ connecting atoms n–1 and n)

$$\mathbf{v}'_{n-1:n+1} = \mathbf{v}_{n-1:n} + \mathbf{T}_{n-1:n:n+1}\left(\psi,\theta\right)\mathbf{v}_{n:n+1} = \mathbf{v}_{n-1:n} + \mathbf{R}_2\left(\psi,\mathbf{x}\right)\mathbf{R}_1\left(-\theta,\mathbf{z}\right)\mathbf{v}_{n:n+1}$$

$$\mathbf{R}_2\left(\psi,\mathbf{x}\right)\mathbf{R}_1\left(-\theta,\mathbf{z}\right)\mathbf{v}_{n:n+1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{bmatrix}\begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} v \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} v\cos\theta \\ v\sin\theta\cos\psi \\ -v\sin\theta\sin\psi \end{bmatrix}$$

Here θ is the supplement of the valence angle formed by atoms n–1, n, and n+1 and ψ is the torsion angle about bond n–1:n.

Matrix representation of chain extension $\mathbf{r}_{1:N}$

The end-to-end vector $\mathbf{r}_{1:N}$ linking terminal atoms is the sum of the bond vectors along the intervening chemical/virtual bonds.

Each virtual bond vector $\mathbf{v}_{i:i+1}$ is initially expressed in the frame of the designated bond (i:i+1).

Consider the sample chain comprised of four atoms (1, 2, 3, 4), three bonds (1:2, 2:3, 3:4) with end-to-end vector $\mathbf{r}_{1:4}$

$$\mathbf{r}_{1:4} = \mathbf{v}_{1:2} + \mathbf{T}_{1:2:3}\,\mathbf{v}_{2:3} + \mathbf{T}_{1:2:3}\,\mathbf{T}_{2:3:4}\,\mathbf{v}_{3:4}$$

The vector sum can alternatively be written as a product of generator matrices, or tensors, with matrix and vector components.

$$\mathbf{r}_{1:4} = \begin{bmatrix} \mathbf{E}_3 & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{T}_{1:2:3} & \mathbf{v}_{1:2} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{T}_{2:3:4} & \mathbf{v}_{2:3} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{T}_{3:4:5} & \mathbf{v}_{3:4} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{r}_{1:4} = \mathbf{J}^{\mathrm{T}}\,\boldsymbol{A}_{12}\,\boldsymbol{A}_{23}\,\boldsymbol{A}_{34}\,\mathbf{J}$$

$$\boldsymbol{A}_{n-1:n} = \begin{bmatrix} \mathbf{T}_{n-1:n:n+1} & \mathbf{v}_{n-1:n} \\ \mathbf{0} & 1 \end{bmatrix}$$

Evaluation of product of chain generator matrices

$$\mathbf{r}_{1:4} = \begin{bmatrix} \mathbf{E}_3 & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{T}_{1:2:3} & \mathbf{v}_{1:2} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{T}_{2:3:4} & \mathbf{v}_{2:3} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{T}_{3:4:5} & \mathbf{v}_{3:4} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{r}_{1:4} = \begin{bmatrix} \mathbf{E}_3 & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4} & \mathbf{T}_{1:2:3}\mathbf{v}_{2:3} + \mathbf{v}_{1:2} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{T}_{3:4:5} & \mathbf{v}_{3:4} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{r}_{1:4} = \begin{bmatrix} \mathbf{E}_3 & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{T}_{3:4:5} & \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{v}_{3:4} + \mathbf{T}_{1:2:3}\mathbf{v}_{2:3} + \mathbf{v}_{1:2} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{r}_{1:4} = \begin{bmatrix} \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{T}_{3:4:5} & \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{v}_{3:4} + \mathbf{T}_{1:2:3}\mathbf{v}_{2:3} + \mathbf{v}_{1:2} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{r}_{1:4} = \mathbf{T}_{1:2:3}\mathbf{T}_{2:3:4}\mathbf{v}_{3:4} + \mathbf{T}_{1:2:3}\mathbf{v}_{2:3} + \mathbf{v}_{1:2}$$

Matrix representation of chain extension

General expression for chain of N atoms.

$$\mathbf{r}_{1:N} = \mathbf{J}^{\mathsf{T}}\, \mathbf{A}_{12}\, \mathbf{A}_{23}\, \mathbf{A}_{34} \cdots \mathbf{A}_{N\text{-}1:N}\, \mathbf{J}$$

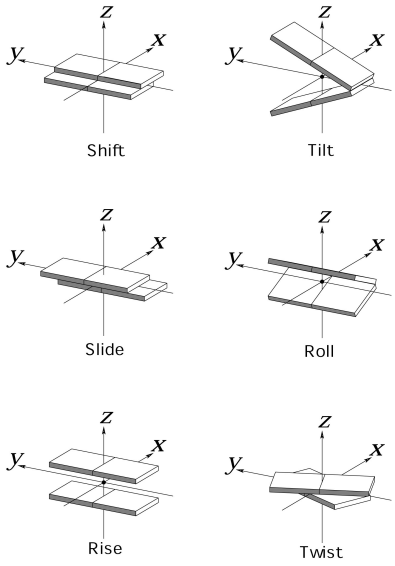
$$\mathbf{J}^{T} = \begin{bmatrix} \mathbf{E}_3 & \mathbf{0} \end{bmatrix} \qquad \mathbf{A}_{i-1:i} = \begin{bmatrix} \mathbf{T}_{i-1:i:i+1} & \mathbf{v}_{i-1:i} \\ \mathbf{0} & 1 \end{bmatrix} \qquad \mathbf{J} = \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}$$

$$\mathbf{J}^{\mathsf{T}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad \mathbf{A}_{i-1:i} = \begin{bmatrix} \cos\theta & \sin\theta & 0 & v \\ -\cos\psi\sin\theta & \cos\psi\cos\theta & -\sin\psi & 0 \\ -\sin\psi\sin\theta & \sin\psi\cos\theta & \cos\psi & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \mathbf{J} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Each chemical/virtual bond vector $\mathbf{v}_{i-1:i}$ is initially expressed in the frame of the designated bond (i:i+1).

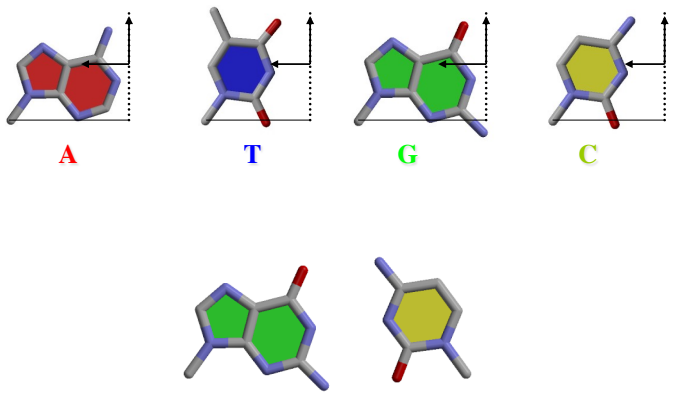
Polymer chain generation in terms of rigid-body parameters

The 3D arrangements of successive base pairs in nucleic acid helices are often described in terms of six rigid-body "step" parameters

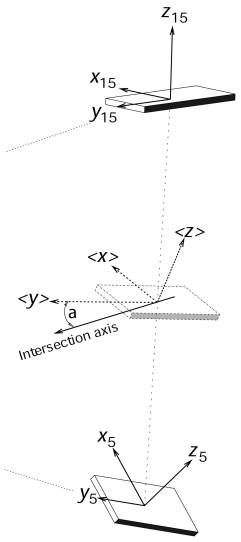


The atoms comprising the bases are located in a "standard" coordinate frame.

The *x*-axis points toward the major groove, the *y*-axis toward the chain backbone, and the *z*-axis forms a right-handed frame, i.e., **z** = **x** × **y**.

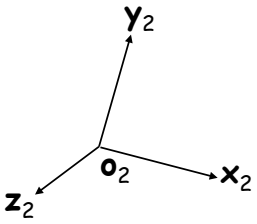


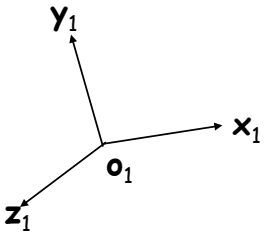
A "middle" frame is used to insure the symmetry of the rigid-body parameters regardless of chain direction.



Characterize spatial relationships between rigid-body frames

Rotation 1: align *y* axis

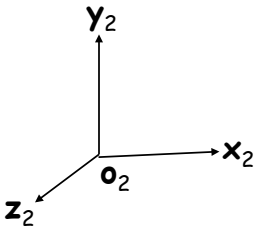


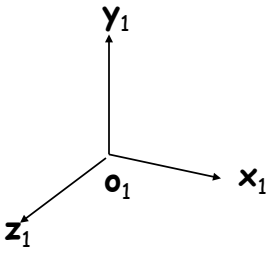


Characterize spatial relationships between rigid-body frames

Rotation 1: align *y* axis

Rotation 2: align *x* and *z* axes

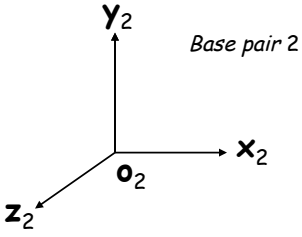


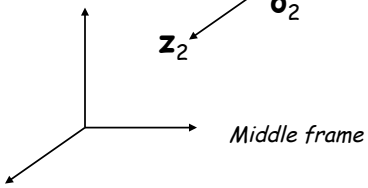


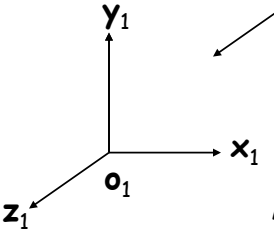
Characterize spatial relationships between rigid-body frames

Rotation 1: align *y* axis

Rotation 2: align *x* and *z* axes







Base pair 1

Parameters are based on a "symmetrized" matrix and "middle" frame.

Angular parameters are incorporated symmetric matrix operations

$$\mathbf{T}_{n:n+1} = \mathbf{Z}\left(\frac{\Omega}{2} - \alpha\right)\mathbf{Y}\left(\beta\right)\mathbf{Z}\left(\frac{\Omega}{2} + \alpha\right)$$

Tilt: $\tau = \beta \sin\alpha$
Roll: $\rho = \beta \cos\alpha$
Twist: Ω

$$\alpha = \left(\tau^2 + \rho^2\right)^{1/2}$$

Zhurkin et al. (1978)
El Hassan & Calladine (1995)

Parameters are based on a "symmetrized" matrix and "middle" frame.

Translational parameters are symmetrized in terms of a "middle" coordinate frame

$$\mathbf{T}_{n:n+1} = \mathbf{Z}\left(\frac{\Omega}{2} - \alpha\right)\mathbf{Y}\left(\frac{\beta}{2}\right)\mathbf{Z}\left(\alpha\right)\mathbf{Z}\left(-\alpha\right)\mathbf{Y}\left(\frac{\beta}{2}\right)\left(\frac{\Omega}{2} + \alpha\right) = \mathbf{T}_{n:m}\mathbf{T}_{m:n+1}$$

Tilt: Dx
Roll: $Dy = \mathbf{T}^{-1}_{n:m}\mathbf{v}_{n:n+1}$
Twist: Dz

Zhurkin et al. (1978)
El Hassan & Calladine (1995)

Matrix elements of $\mathbf{T}_{n,n+1} = \mathbf{Z}(\Omega/2-a)\mathbf{Y}(\beta)\mathbf{Z}(\Omega/2+a)$

$$\begin{bmatrix} \cos\beta\cos\left(\alpha-\frac{\Omega}{2}\right)\cos\left(\alpha+\frac{\Omega}{2}\right)+\sin\left(\alpha-\frac{\Omega}{2}\right)\sin\left(\alpha+\frac{\Omega}{2}\right) & -\cos\beta\cos\left(\alpha-\frac{\Omega}{2}\right)\sin\left(\alpha+\frac{\Omega}{2}\right)+\sin\left(\alpha-\frac{\Omega}{2}\right)\cos\left(\alpha+\frac{\Omega}{2}\right) & \sin\beta\cos\left(\alpha-\frac{\Omega}{2}\right) \\ -\cos\beta\sin\left(\alpha-\frac{\Omega}{2}\right)\cos\left(\alpha+\frac{\Omega}{2}\right)+\cos\left(\alpha-\frac{\Omega}{2}\right)\sin\left(\alpha+\frac{\Omega}{2}\right) & \cos\beta\sin\left(\alpha-\frac{\Omega}{2}\right)\sin\left(\alpha+\frac{\Omega}{2}\right)+\cos\left(\alpha-\frac{\Omega}{2}\right)\cos\left(\alpha+\frac{\Omega}{2}\right) & -\sin\beta\sin\left(\alpha-\frac{\Omega}{2}\right) \\ -\sin\beta\cos\left(\alpha+\frac{\Omega}{2}\right) & \sin\beta\sin\left(\alpha+\frac{\Omega}{2}\right) & \cos\beta \end{bmatrix}$$

Step parameters are obtained by equating matrix elements to numerical values extracted from Cartesian coordinates of given structure, *e.g.*, cos β = $\mathbf{T}_{i,i+1}(3,3)$

w3DNA application

Rebuilding: customized base-pair step/nucleotide parameters

The pathway of an ideal DNA superhelix of n_{bp} can be generated from the following rigid-body parameters:

$$\text{Tilt (deg)} = \left(\frac{360}{n_{bp}}\right)\cos\left(36(m-0.5)\right)$$

$$\text{Roll (deg)} = \left(\frac{360}{n_{bp}}\right)\cos\left(36(m-0.5)+90\right)$$

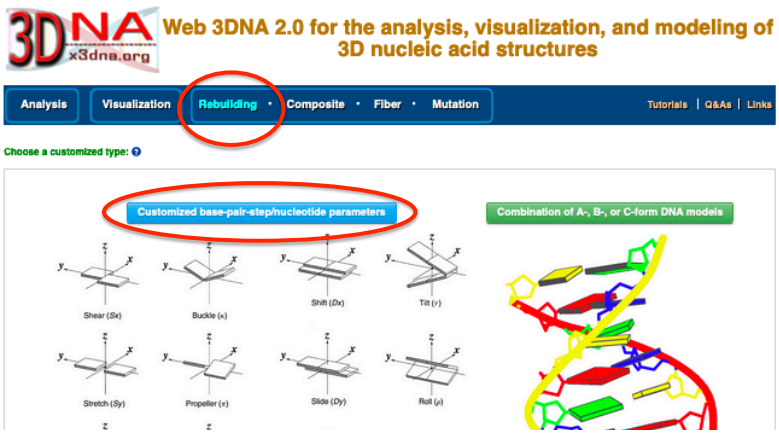
$$\text{Twist} = \frac{360}{n_{bp}}$$

Shift = 0Å
Slide = 0 Å
Rise = 3.4 Å

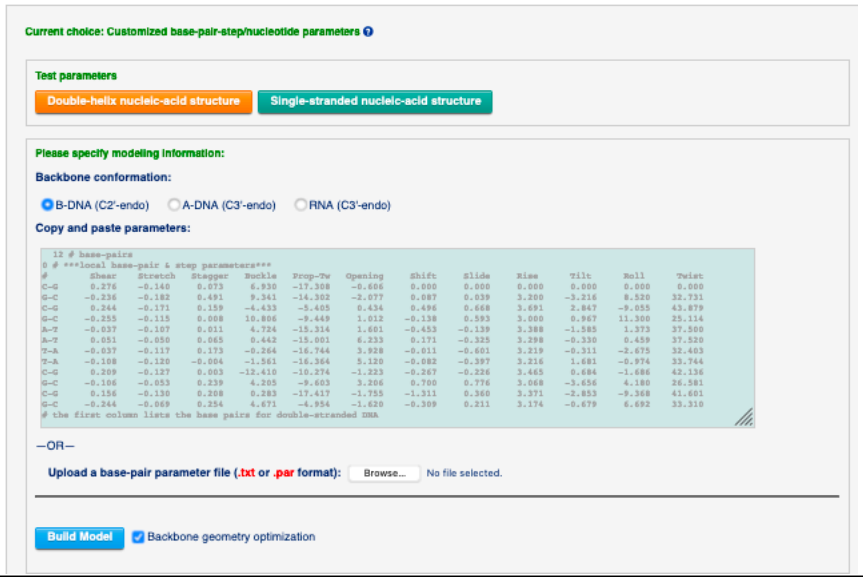
Here the angles are expressed in degrees and m is the index of the base-pair step. The choice of n_{bp} alters the pitch of the assembly.

http://web.x3dna.org/

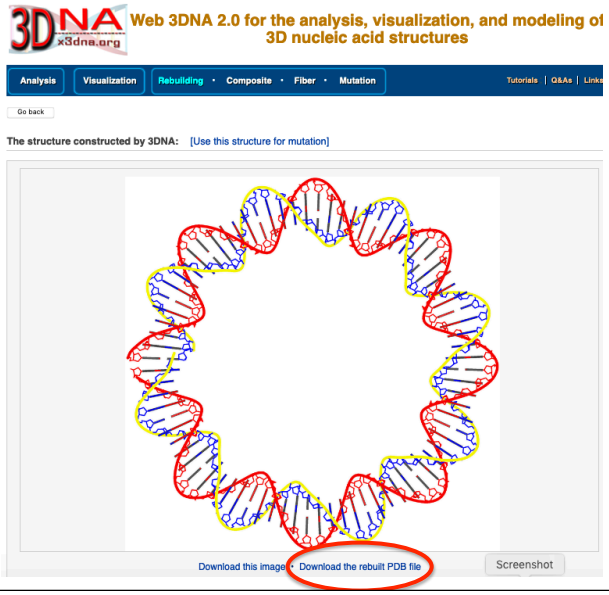
The w3DNA Rebuilding module includes an option to construct models of DNA or RNA from the rigid-body parameters that describe the 3D arrangements of coordinate frames on paired bases and successive base pairs or nucleosomes.



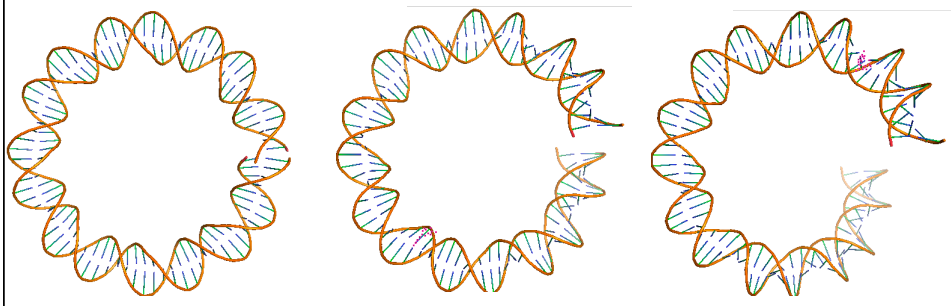
The rigid-body parameters can be entered or selected with the browser option.



A Protein Data Bank-formatted file of the generated structure can be downloaded from the webserver.



Pathways illustrating how the choice of n_{bp} affects the pitch of ideal, 80-bp DNA superhelices



n_{bp}=10 n_{bp}=10.2 n_{bp}=10.4