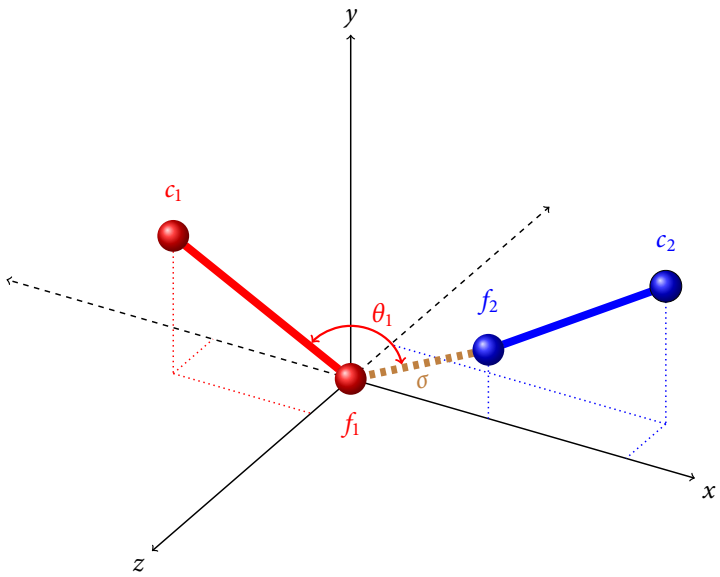
1 Theta



Definitions:

$\hat{\boldsymbol{v}} = f_1 - c_1$, the center of mass to reacting interface vector for reactant molecule 1

$\hat{\boldsymbol{\sigma}} = f_2 - f_1$, vector between the two reacting interfaces

θ: angle between the $\hat{\boldsymbol{v}}$ and $\hat{\boldsymbol{\sigma}}$

angle range: $[0, \pi]$

Procedure:
Note that each reacting molecule is associated to a separate θ angle. The indices 1 and 2 refer to the molecule to whom the θ angle belongs to and the other molecule, respectively.

1. Determine angle to rotate each complex by
   (a) Calculate current angle, θ_{curr}
   $$\theta_{\text{curr}} = \arccos\left(\frac{\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{\sigma}}}{|\hat{\boldsymbol{v}}||\hat{\boldsymbol{\sigma}}|}\right)$$
   (b) Determine difference from the target angle, θ_{targ}, $\theta_{\text{rot}} = \theta_{\text{targ}} - \theta_{\text{curr}}$
   (c) Determine the angle to rotate each complex by (the complexes are rotated in opposite directions), according to their diffusion rotation constants,
   $$\theta_{\text{pos.}} = \begin{Bmatrix} \frac{1}{2}\left(\theta_{\text{targ}} - \theta_{\text{curr}}\right) & \text{if } Dr_z^{\text{dom.}} = 0 \\ \frac{Dr_z}{Dr_{\text{tot}}}\left(\theta_{\text{targ}} - \theta_{\text{curr}}\right) & \text{if } Dr_z^{\text{dom.}} \neq 0 \end{Bmatrix}$$
   $$\theta_{\text{neg.}} = \begin{Bmatrix} -\theta_{\text{pos.}} & \text{if } Dr_z^{\text{inf}} = 0 \\ \frac{Dr_z}{Dr_{\text{tot}}}\left(\theta_{\text{targ}} - \theta_{\text{curr}}\right) & \text{if } Dr_z^{\text{inf.}} \neq 0 \end{Bmatrix}$$
   (d) If $\theta_{\text{targ.}} - \theta_{\text{curr.}} < 1e^{-8}$, no rotation is done for this angle.
2. Determine rotation axis (this could probably be simplified to just use $\hat{\boldsymbol{x}}$ or $\hat{\boldsymbol{y}}$ instead of $\hat{\boldsymbol{v}} \times \hat{\boldsymbol{x}}$ or $\hat{\boldsymbol{v}} \times \hat{\boldsymbol{y}}$),
   $$\hat{\boldsymbol{u}} = \begin{Bmatrix} \hat{\boldsymbol{v}} \times \hat{\boldsymbol{x}} & \text{if } (\theta_{\text{curr.}} = 0 \,||\, \theta_{\text{curr.}} = \pi) \;\&\; (\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{x}} \neq 0 \;\&\; \hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{x}} \neq \pi) \\ \hat{\boldsymbol{v}} \times \hat{\boldsymbol{y}} & \text{if } (\theta_{\text{curr.}} = 0 \,||\, \theta_{\text{curr.}} = \pi) \;\&\; (\hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{x}} = 0 \,||\, \hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{x}} = \pi) \\ \hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{v}} & \text{otherwise} \end{Bmatrix}$$

3. Set up rotation quaternions, which are then normalized,

$$Q_{\text{pos.}} = \cos\left(\frac{\theta_{\text{pos..}}}{2}\right) + \left[\sin\left(\frac{\theta_{\text{pos.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{x}}\right]\hat{\boldsymbol{i}} + \left[\sin\left(\frac{\theta_{\text{pos.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{y}}\right]\hat{\boldsymbol{j}} + \left[\sin\left(\frac{\theta_{\text{pos.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{z}}\right]\hat{\boldsymbol{k}}$$

$$Q_{\text{neg.}} = \cos\left(\frac{\theta_{\text{neg..}}}{2}\right) + \left[\sin\left(\frac{\theta_{\text{neg.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{x}}\right]\hat{\boldsymbol{i}} + \left[\sin\left(\frac{\theta_{\text{neg.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{y}}\right]\hat{\boldsymbol{j}} + \left[\sin\left(\frac{\theta_{\text{neg.}}}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{z}}\right]\hat{\boldsymbol{k}}$$

4. Iterate over all vectors, (dominant interface)–(x), where x is every other center of mass/interface coordinate, and rotate with $Q_{\text{pos.}}$ for the dominant complex and $Q_{\text{neg.}}$ for the inferior complex,

$$\hat{\boldsymbol{v}}_{\text{rot.}} = Q_{\text{i}}\left(\hat{\boldsymbol{v}}\right) Q_{\text{i}}^{-1}$$

- When doing this, $\hat{\boldsymbol{v}}$ is a quaternion with w component of 0.
- Q^{-1} is the inverse quaternion,

$$Q^{-1} = \frac{\left[Q_w - Q_x\hat{\boldsymbol{i}} - Q_y\hat{\boldsymbol{j}} - Q_z\hat{\boldsymbol{k}}\right]}{|Q|}$$

- Quaternion multiplication:

$$\begin{aligned} Q_{\text{new}} = &\left[\left(Q_{1,w} * Q_{2,w}\right) - \left(Q_{1,x} * Q_{2,x}\right) - \left(Q_{1,y} * Q_{2,y}\right) - \left(Q_{1,z} * Q_{2,z}\right)\right] \\ &+ \left[\left(Q_{1,w} * Q_{2,x}\right) + \left(Q_{1,x} * Q_{2,w}\right) + \left(Q_{1,y} * Q_{2,z}\right) - \left(Q_{1,z} * Q_{2,y}\right)\right]\hat{\boldsymbol{i}} \\ &+ \left[\left(Q_{1,w} * Q_{2,y}\right) + \left(Q_{1,y} * Q_{2,w}\right) + \left(Q_{1,z} * Q_{2,x}\right) - \left(Q_{1,x} * Q_{2,z}\right)\right]\hat{\boldsymbol{j}} \\ &+ \left[\left(Q_{1,w} * Q_{2,z}\right) + \left(Q_{1,z} * Q_{2,w}\right) + \left(Q_{1,x} * Q_{2,y}\right) - \left(Q_{1,y} * Q_{2,x}\right)\right]\hat{\boldsymbol{k}} \end{aligned}$$

2 Phi

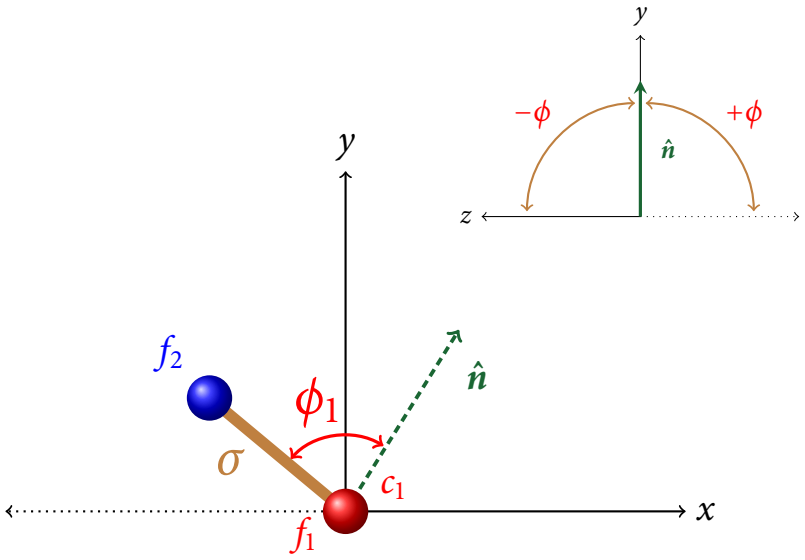


Figure 1: Definition of phi angle, the dihedral (torsion) angle between a predefined vector, $\hat{\boldsymbol{n}}$ and the interface to interface vector, $\hat{\boldsymbol{\sigma}}$. The sign of the angle is determined by the position of vector $\hat{\boldsymbol{n}}$ relative to vector $\hat{\boldsymbol{\sigma}}$, shown in the inset.

Definitions:

$\hat{\boldsymbol{\sigma}} = f_2 - f_1$, the vector between the two reacting interfaces

$\hat{\boldsymbol{n}}$: normal of the molecule, as given by the user (usually the z or y principle axis)

ϕ_i: dihedral angle between $\hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{n}}$

angle range: $[\pi, -\pi]$

Procedure:
Note that each reacting molecule is associated to a separate ϕ angle. The indices 1 and 2 refer to the molecule to whom the ϕ angle belongs to and the other molecule, respectively.

1. Determine the current angle, $\phi_{\text{curr.}}$, through an orthographic projection onto the xy plane

   (a) Transform the molecule such that the axis of rotation, $\hat{\boldsymbol{v}}$, is aligned with the z axis

   - Get angle between the current $\hat{\boldsymbol{\sigma}}$ and the z axis,

$$\chi = \arccos\left(\frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{z}}}{|\hat{\boldsymbol{\sigma}}||\hat{\boldsymbol{z}}|}\right)$$

   - Get the rotation axis, $\hat{\boldsymbol{u}} = \hat{\boldsymbol{\sigma}} \times \hat{\boldsymbol{z}}$
   - Create quaternion and rotate,

$$Q = \cos\left(\frac{\chi}{2}\right) + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_x\right]\hat{\boldsymbol{i}} + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_y\right]\hat{\boldsymbol{j}} + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_z\right]\hat{\boldsymbol{k}}$$

   (b) In the transformed coordinate system, get the two vectors, $\hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{n}}$. The vector $\hat{\boldsymbol{n}}$ must be determined through a rotation to fit the coordinates to the provided molecule template internal coordinates, to obtain the current orientation (a dummy particle would be too computationally expensive).

i. Center the molecule to origin $(0, 0, 0)$ by subtracting all coordinates by the center of mass.

ii. Get the angle (μ_1) between $\hat{\boldsymbol{f}}_{\text{curr.}} = f_{\text{curr.}} - c_{\text{curr.}}$, the current center of mass to reacting interface vector, and $\hat{\boldsymbol{f}}_{\text{targ.}} = f_{\text{targ.}} - c_{\text{targ.}}$, the center of mass to reacting interface vector provided by the user

iii. Create the rotation quaternion,

$$Q_1 = \cos\left(\frac{\mu_1}{2}\right) + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{x}}\right]\hat{\boldsymbol{i}} + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{y}}\right]\hat{\boldsymbol{j}} + \left[\sin\left(\frac{\mu_1}{2}\right) * \hat{\boldsymbol{u}}_{\boldsymbol{z}}\right]\hat{\boldsymbol{k}}$$

where $\hat{\boldsymbol{u}} = \hat{\boldsymbol{f}}_{\text{targ.}} \times \hat{\boldsymbol{f}}_{\text{curr.}}$.

iv. Rotate the molecule using this quaternion, as described above.

v. If the molecule has more than one interface, repeat this process using the second interface, obtaining Q_2.

vi. Return the quaternion,

$$Q_{\text{rot}}^{\hat{\boldsymbol{n}}} = \begin{Bmatrix} Q_1 & \text{if interfaces} = 1 \\ Q_2 Q_1 & \text{otherwise} \end{Bmatrix}$$

vii. Rotate the provided normal with $Q_{\text{rot.}}^{\hat{\boldsymbol{n}}}$ to obtain the current normal, $\hat{\boldsymbol{n}}$

(c) Still in the transformed coordinate system, project $\hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{n}}$ onto the xy plane. For example,

$$\hat{\boldsymbol{\sigma}}_{\text{proj.}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{\sigma}}_{\boldsymbol{x}} \\ \hat{\boldsymbol{\sigma}}_{\boldsymbol{y}} \\ \hat{\boldsymbol{\sigma}}_{\boldsymbol{z}} \end{bmatrix} = \begin{bmatrix} \hat{\boldsymbol{\sigma}}_{\boldsymbol{x}} \\ \hat{\boldsymbol{\sigma}}_{\boldsymbol{y}} \\ 0 \end{bmatrix}$$

(d) Get ϕ by the dot product,

$$\phi = \arccos\left(\frac{\hat{\boldsymbol{\sigma}}_{\text{proj.}} \cdot \hat{\boldsymbol{n}}_{\text{proj.}}}{|\hat{\boldsymbol{\sigma}}_{\text{proj.}}||\hat{\boldsymbol{n}}_{\text{proj.}}|}\right)$$

2. Do steps 1b through 4 for the θ rotation, replacing all angle calculations with the above procedure for ϕ

3 Omega

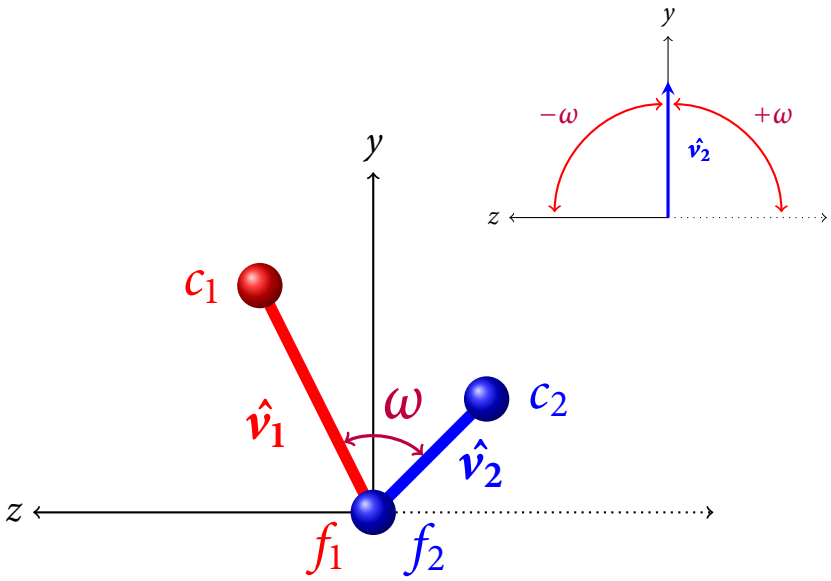


Figure 2: Definition of omega angle, comprised of the two reacting interface to center of mass vectors ($\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$) for each molecule. The sign of the angle is determined by the position of vector $\hat{\mathbf{v}}_1$ relative to vector $\hat{\mathbf{v}}_2$, shown in the inset.

Definitions:

$\hat{\mathbf{v}}_1$: $f_1 - c_1$, center of mass to reacting interface vector for reactant molecule 1

$\hat{\mathbf{v}}_2$: $f_2 - c_2$, center of mass to reacting interface vector for reactant molecule 2

$\hat{\mathbf{n}}_1$: the normal of reactant molecule 1, provided by the user

$\hat{\mathbf{n}}_2$: the normal of reactant molecule 2, provided by the user

$\hat{\boldsymbol{\sigma}}$: $f_2 - f_1$, vector between the two reacting interfaces (current complex's interface to other complex's interface)

ω: dihedral between the $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$, *or* the dihedral between the normals of the two reacting molecules

angle range: $[\pi, -\pi]$

Procedure:

1. Follows the same procedure for the ϕ rotation, replacing $\hat{\boldsymbol{n}}$ and $\hat{\boldsymbol{\sigma}}$ with one of two sets of vectors:

$$\begin{Bmatrix} \hat{\mathbf{n}}_1, \hat{\mathbf{n}}_2 & \text{if } \theta_1 = \pi \,||\, \theta_2 = \pi \\ \hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2 & \text{otherwise} \end{Bmatrix}$$

   This is necessary since if either θ angle is equal to π, the dihedral between $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ is undefined, but an equivalent dihedral could still be necessary to properly align the two molecules (such as in the case of two planar clathrins associating)