

1 Cyclic polygon expansion plane

The plane that the cyclic polygon expands into can be found as follows:

We define the dihedral atom sequence $\vec{A}, \vec{B}, \vec{C}, \vec{D}$ with the angles $\alpha = \angle ABC, \beta = \angle BCD$ and the dihedral $\varphi = \angle ABCD$ with the following conditions:

$$|AB| = a, |BC| = b, |CD| = c$$

$$\alpha, \beta \in [0, \pi], \varphi \in [-\pi, \pi]$$

We arbitrarily choose the following positions for the points:

$$\vec{A} = \mathbf{R}_z(\alpha)a\vec{e}_x \quad (1)$$

$$\vec{B} = \vec{0} \quad (2)$$

$$\vec{C} = b\vec{e}_x \quad (3)$$

$$\vec{D} = \mathbf{R}_x(\varphi) \left[\vec{C} + \mathbf{R}_z(\pi - \beta)c\vec{e}_x \right] \quad (4)$$

where \vec{e}_x is the unit vector along the x axis and \mathbf{R}_i is the rotation matrix along the axis i .

The dihedral distance is formed by the line segment \overline{AD} .

In order to find the shortest distance between the line segments \overline{AD} and \overline{BC} , we define:

$$\overline{BC} : \vec{r}(\lambda) = \vec{B} + \lambda(\vec{C} - \vec{B}) = \lambda\vec{C}, \lambda \in [0, 1] \quad (5)$$

$$\overline{AD} : \vec{s}(\mu) = \vec{A} + \mu(\vec{D} - \vec{A}), \mu \in [0, 1] \quad (6)$$

The shortest distance between the line segments must be orthogonal to both line segments' direction vectors:

$$\left[\lambda\vec{C} - (\vec{A} + \mu(\vec{D} - \vec{A})) \right] \cdot \vec{C} = 0 \quad (7)$$

$$\left[\lambda\vec{C} - (\vec{A} + \mu(\vec{D} - \vec{A})) \right] \cdot (\vec{D} - \vec{A}) = 0 \quad (8)$$

Solving this system of equations yields:

$$\mu_0 = -\frac{A_y S_y + A_z S_z}{S_y^2 + S_z^2} \quad (9)$$

$$\lambda_0 = \frac{A_x + \mu_0 S_x}{b} \quad (10)$$

$$\text{with } \vec{S} = \vec{D} - \vec{A} \quad (11)$$

These do not satisfy their conditions yet:

$$\lambda_m = \min(\max(\lambda_0, 0), 1) \quad (12)$$

$$\mu_m = \begin{cases} -\frac{A_x}{S_x} & \lambda_0 \leq 0 \\ \frac{b-A_x}{S_x} & \lambda_0 \geq 1 \\ \lambda_0 & \text{else} \end{cases} \quad (13)$$

The plane in which the cyclic polygon expands can then be defined via the three points \vec{A}, \vec{D} , and $\vec{r}(\lambda_m)$.

For $\varphi = \pm\pi$, these points become collinear and the plane definition is invalid. Under these circumstances, the plane can instead be defined using the point \vec{A} and the two vectors $(\vec{D} - \vec{A})$ and \vec{e}_z .