# Monte Carlo simulations of circular supercoiled polymers

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## 1 Intersections

Monte Carlo moves can result in regions of the polymer intersecting between each other. To prevent this movement to occurs we need to check if the resulting trial configuration is intersecting. Then, a pair of edges of the polymer is defined by the following equations:

$$\vec{r} = \vec{r}_0 + \delta_1 \hat{t} \tag{1}$$

$$\vec{u} = \vec{u}_0 + \delta_2 \hat{v} \tag{2}$$

where $\vec{r}_0$ and $\vec{u}_0$ are the coordinates of the two points of the polymer and $\hat{t}$ and $\hat{v}$ are the local and unitary direction vectors. The squared distance between the two lines is $d(\vec{r}, \vec{u}) = \|\vec{r} - \vec{u}\|^2$ and we look for the $\delta_1$ and $\delta_2$ minimising the distance $d$,

$$\frac{\partial d(\vec{r}, \vec{u})}{\partial \delta_1} \stackrel{!}{=} 0, \qquad \frac{\partial d(\vec{r}, \vec{u})}{\partial \delta_2} \stackrel{!}{=} 0 \tag{3}$$

Evaluating the derivatives and solving for $\delta_i$, we find,

$$\boxed{\delta_2 = \frac{(\vec{r}_0 - \vec{u}_0) \cdot \hat{v} - [(\vec{r}_0 - \vec{u}_0) \cdot \hat{v}](\hat{t} \cdot \hat{v})}{(\hat{t} \cdot \hat{v})^2 - 1}} \tag{4}$$

and

$$\boxed{\delta_1 = \delta_2 (\hat{t} \cdot \hat{v}) - (\vec{r}_0 - \vec{u}_0) \cdot \hat{t}} \tag{5}$$

We check if $0 < \delta_1 < s_1$ and $0 < \delta_2 < s_2$, with $s_i$ the length of the edges. If $\delta_1$ and $\delta_2$ are in the indicated range, then the minimum distance between points is occuring at some point along the edges defined at $\vec{r}_0$ and $\vec{u}_0$. In such scenario, we check if $d(\vec{r}, \vec{u})\big|_{\delta_1, \delta_2} < 2R$, with $R$ the (effective) polymer radius: in affirmative case, there is an intersection at the edge.

The indicated procedure is repeated for every possible pair of edges. Hence, this is a complex step, with a complexity order $\mathcal{O} \sim N^2$, with $N$ the number of edges/particles.

## 2 Knots

Fáry–Milnor theorem