Calculating binding site position from minus end for partical cylinders given α (binding position from first monomer) **MEDYANv4.2**β

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1 Overview

In MEDYAN, linker/motor and brancher binding sites on a cylinder are stored as binding site fractions referred in this document as α. Binding site fraction, stored in **CBound** object as *_position1* and *_position2* measures the fraction of distance from first monomer of the cylinder in a cylinder of N monomers.

1.1 Full vs Partial Cylinders

Full cylinders are N monomers in length. Partial cylinders span monomers $x - y$, where $x > 1$ and $y < N$.

1.2 Usage of α in Chemical Objects

CLinker, CMotorGhost, and CBranchingPoint classes use α to determine the monomer to which they are bound ($M_{bound} = \alpha \times N \epsilon [1, N]$). Even partial cylinders have an array size of N and so, this parameter can be used directly.

1.3 Usage of α in Mechanical Objects

MLinker, MMotorGhost, and MBranchingPoint objects currently use α parameter to determine the coordinate of bound molecule along any cylinder. α is defined as shown in

Fig.1A. Currently, MEDYAN codes use this value to determine coordinate of the molecule along the cylinder. This is problematic for partial cylinders as the binding site is assumed to be at $\alpha \times L_{cyl}$ from the x^{th} monomer. To correct for this discrepancy, a method implementation is made in **Cylinder** class.
The function `adjustedrelativeposition` takes α as the input and determines corrected α^{corr} such that the coordinate specified at $\alpha^{corr} \times L_{cyl}$ distance from first monomer matches with the coordinate specified at $\alpha \times L_{full}$ measured from x^{th} monomer.

2 Obtain expression for α^{corr} from α

Consider the partial cylinder shown in Fig. 1. The corrected parameter $alpha^{corr}$ is obtained as follows.

$$\alpha = \frac{L_{bind}}{L_{full}} \tag{1}$$

$$= \frac{L_m + L1}{L_{full}} = \frac{\frac{L_m}{L_{cyl}} + \frac{L1}{L_{cyl}}}{\frac{L_{full}}{L_{cyl}}} \tag{2}$$

$$\alpha = \frac{\frac{L_m}{L_{cyl}} + \alpha^{corr}}{\frac{L_{full}}{L_{cyl}}} \tag{3}$$

$$\alpha^{corr} = \frac{\alpha L_{full}}{L_{cyl}} - \frac{L_m}{L_{cyl}} \tag{4}$$

Similarly, one can also define a definition from $1 - \alpha$.

$$1 - \alpha = \frac{L_p + L2}{L_{full}} = \frac{\frac{L_p}{L_{cyl}} + \frac{L2}{L_{cyl}}}{\frac{L_{full}}{L_{cyl}}} \tag{5}$$

$$= \frac{\frac{L_p}{L_{cyl}} + (1 - \alpha^{corr})}{\frac{L_{full}}{L_{cyl}}} \tag{6}$$

$$\alpha^{corr} = 1 - (1 - \alpha)\frac{L_{full}}{L_{cyl}} + \frac{L_p}{L_{cyl}} \tag{7}$$

2.1 Special cases

Consider a **plus end cylinder** (last cylinder in a multi-cylinder filament, or x≥1, y=N, y-x+1≤ N). Using Eq. (4), we substitute $L_m = 0$, to get, $\alpha^{corr} = \frac{\alpha L_{full}}{L_{cyl}}$.
Consider a **minus end cylinder** (first cylinder in a multi-cylinder filament, or x=1, y≤N, y-x+1≤N). Using Eq. (7), we substitute $L_p = 0$, to get, $\alpha^{corr} = 1 - (1 - \alpha)\frac{L_{full}}{L_{cyl}}$.

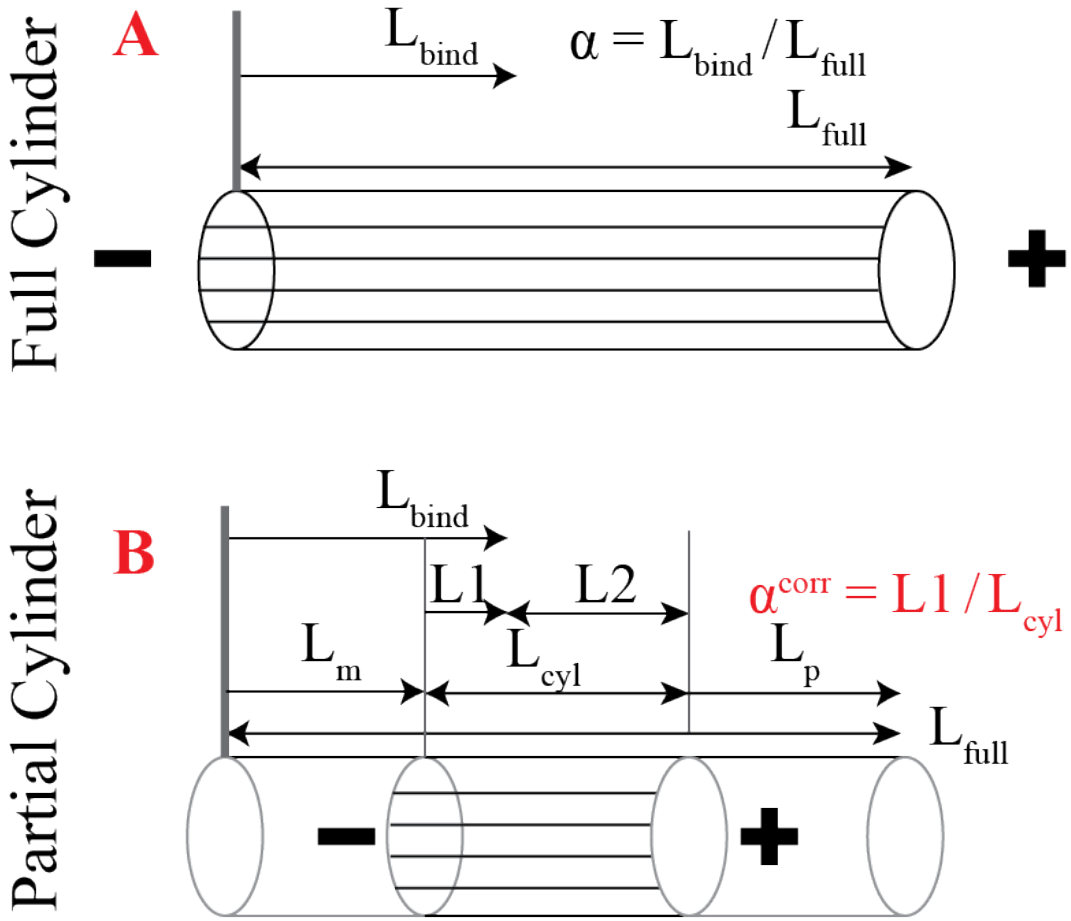

Figure 1: **Schematic outlining α and α^{corr} (A)** shows a full length cylinder along with the definition of α
. **(B)** shows a partial cylinder along with the parameter required by mechanical objects α^{corr}. Partial cylinder spans monomers $x - y$, where $x > 1$ and $y < N$. In the above schematic, L_{bind} refers to the distance of binding site from the first minus end monomer, L_{full} refers to the maximum allowed length for a cylinder (specified in systeminput file), while L_{cyl} refers to the length of partial cylinder. L_m/L_p refer to the distance of minus end (plus end) from first (N^{th}) monomer. In panel **B**, $L_{cyl} = L1 + L2$ and $L_{bind} = L_m + L1$.