Creating looped Polymer by Brownian Bridges- implications for polymer dynamics simulations

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Given a linear polymer of N beads, and a set of pairs of bead indices to connect into loops, we use the Brownian bridge transformation on the linear polymer to iteratively loop it accordingly. Since a random initial configuration of the Gaussian chain does not differ by its random configuration after relaxation time, we can save simulation time by starting with a looped polymer.

First, some terms. The indices of a begining and end of loop form an interval on the linear polymer. This interval can either contain or be contained by other intervals, contain the start/end index of another interval, or not contain any other interval.

The procedure goes as follows

1. classify the loops to those containing other loops and those who don't.

2.

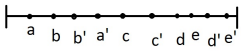

Figure 1: four types of intervals. [a a'] contains [b b'], [c c'] is not contained, [d d'] contains the start of [e e']