Bubble merging in breathing DNA as a vicious walker problem in opposite potentials - DTU Orbit (16/01/2019)

Bubble merging in breathing DNA as a vicious walker problem in opposite potentials
We investigate the coalescence of two DNA bubbles initially located at weak domains and separated by a more stable barrier region in a designed construct of double-stranded DNA. In a continuum Fokker-Planck approach, the characteristic time for bubble coalescence and the corresponding distribution are derived, as well as the distribution of coalescence positions along the barrier. Below the melting temperature, we find a Kramers-type barrier crossing behavior, while at high temperatures, the bubble corners perform drift diffusion toward coalescence. In the calculations, we map the bubble dynamics on the problem of two vicious walkers in opposite potentials. We also present a discrete master equation approach to the bubble coalescence problem. Numerical evaluation and stochastic simulation of the master equation show excellent agreement with the results from the continuum approach. Given that the coalesced state is thermodynamically stabilized against a state where only one or a few of the base pairs of the barrier region are re-established, it appears likely that this type of setup could be useful for the quantitative investigation of thermodynamic DNA stability data as well as the rate constants involved in the unzipping and zipping dynamics of DNA in single molecule fluorescence experiments.

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