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Investigating the mechanism of DNA bulk hybridization with Forward Flux Sampling DANIEL HINCKLEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — DNA has become increasingly common as a building block for constructing nanomaterials. However, the mechanism by which DNA hybridization occurs is largely unknown, even in the bulk. Previous work using Transition Path Sampling and a coarse grain DNA model has shown that DNA bulk hybridization occurs via a "slithering" mechanism for repetitive sequences and a distinct nucleation event for random sequences. This mechanistic description remains somewhat incomplete as only configurations within the general vicinity of the transition state ensemble have been examined. In this work, we use Forward Flux Sampling and Langevin Dynamics to examine configurations along the entire transition pathway. We find that, for random sequences, barriers to hybridization arise at certain points in the hybridization pathway requiring reorientation of the two strands. Such barriers are not as pronounced for repetitive sequences where rearrangement occurs without the large scale disruption of hydrogen bonding. The formalism which we use has allowed us to calculate reaction constants for hybridization that are consistent with experiments. It has also allowed us to explain the precipitous decay of reaction rates that is observed when molecular weight is increased.

Daniel Hinckley
Department of Chemical and Biological Engineering,
University of Wisconsin-Madison

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