1093-92-348 **Robert S Manning*** (rmanning@haverford.edu), Mathematics Department, Haverford College, 370 Lancaster Ave., Haverford, PA 19041. *Monte Carlo simulations of DNA cyclization using a rigid-base model and mechanical properties derived from molecular dynamics.* Preliminary report.

A cyclization J-factor is an experimental measurement on short DNA (50-500 basepairs) related to the propensity of the DNA to form a loop. It has proven to be a useful experimental measurement because it depends sensitively on key mechanical properties of the DNA, such as intrinsic bend, intrinsic twist, and twist and bend flexibility. A mathematical quantity key to understanding cyclization J-factors is the end-to-end probability density function (pdf) on $R^3 \times SO(3)$, the configuration space for the far end of the DNA, once the near end is fixed by choice of coordinates. Monte Carlo simulations allow direct sampling of this pdf, although the typical values of the pdf are small enough that it can be challenging to get decent statistics.

We apply the Monte Carlo technique within a DNA model developed in the laboratory of John Maddocks. This model assumes the DNA bases are rigid (but the two bases within a basepair can move relative to each other). The shape and flexibility of the DNA depends on its sequence, through parameters extracted by Maddocks and co-authors by fitting to a large ensemble of molecular dynamics simulations. We present results illustrating how the cyclization J-factor depends on DNA length and on the specific basepair sequence of the DNA. (Received August 20, 2013)