Abstract: Here are some natural questions from statistical physics: What is the expected shape of a ring polymer with $n$ monomers in solution? What is the expected knot type of the polymer? The radius of gyration? Numerical simulations are absolutely required to make progress on these questions, but pose some interesting challenges for geometers.

We wish to sample the space of closed $n$-gons in 3-space, which is a nonlinear submanifold of the larger space of open $n$-gons. To sample equilateral polygon space, current algorithms use a Markov process which randomly "folds" polygons while preserving closure and edgelengths. Such algorithms are expected to converge in $O(n^3)$ time.

The main point of this talk is that a much better sampling algorithm is available if we widen our view to the space of $n$-gons in three dimensional space of fixed total length (rather than fixed edgelengths). We describe a natural probability measure on length $2n$-gon space pushed forward from the standard measure on the Stiefel manifold of 2-frames in complex $n$-space using methods from algebraic geometry. We can directly sample the Stiefel manifold in $O(n)$ time, allowing us to generate closed polygons using the pushforward map.

We will give some explicit computations of expected values for geometric properties for such random polygons, discuss their topology, and compare our theorems to numerical experiments using our sampling algorithm. The talk describes joint work with Malcolm Adams (University of Georgia, USA), Tetsuo Deguchi (Ochanomizu University, Japan), and Clay Shonkwiler (University of Georgia, USA).

Tuesday, January 29, 2013, 4:00 pm
Mathematics and Science Center: W306

Mathematics and Computer Science
Emory University