1139-53-572 Jason Cantarella, Philipp Reiter and Clayton Shonkwiler* (clay@shonkwiler.org),
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80523. A Natural Map from Random Walks to Equilateral Polygons in Any Dimension.

There is a long history of modeling biopolymers by random walks. Such walks exhibit the same scaling behavior as polymers at the $\theta$ temperature, but modeling polymers with nontrivial topology presents additional challenges. Recently, the toric symplectic structure on equilateral polygons in 3 -space has been exploited to give fast sampling algorithms and useful numerical integration techniques, giving the first provably correct method for simulating random walks with nontrivial topology.

Unfortunately, this structure is special to three dimensions: it's due to the equivalence of the 2 -sphere and the complex projective line. Even in the plane, it is challenging to sample equilateral polygons. I will present a map from random walks to closed polygons in any dimension. Viewing the edges of an equilateral polygon as a point cloud on the sphere, the key idea is a proof that the closest closed polygon to an open chain is given by recentering the cloud at its geometric median and renormalizing. This gives a loop closure procedure which is a mathematically principled way to associate a unique closed loop (and knot type) to open chains like proteins. Since sampling points on the sphere is easy, this provides a way of generating large ensembles of closed equilateral polygons. (Received February 19, 2018)

