

# **Modeling Freely Jointed Ring Polymers (and Topological Polymers) with Conformal Barycenter Sampling.**

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## Abstract

In the freely jointed chain model, monomers are connected by edges of fixed lengths joined at vertices, without any constraint on the angles between edges at the vertices. Modeling freely jointed chains numerically has traditionally been difficult, as the edgelength constraints lead to a complicated sample space. In previous work, Cantarella, Deguchi, Duplantier, Shonkwiler and Uehara introduced an algorithm for sampling equilateral freely-jointed rings in 3 dimensions using ideas from symplectic geometry. In this paper, we present a different approach to sampling freely jointed rings which is more flexible. The new method allows us to handle chains whose lengths have different edges and to sample rings in any dimension, including the previously difficult case of planar rings. It is fast and accurate reweighted sampler, with good control on the relative sizes of the sample weights. We will also present some preliminary results on reweighted sampling of freely jointed networks, where the vertices of a "structure graph" are connected by chains of equal length edges. This talk is joint work with Henrik Schumacher (Chemnitz) and Clayton Shonkwiler (Colorado State).