

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

In silico simulations of polymer condensation: the fractal globule as a metastable state¹ LEON FURCHTGOTT*, ASHOK CUTKOSKY*, NAJEEB TARAIZI, Harvard University, EREZ LIEBERMAN AIDEN, Harvard Society of Fellows — The fractal globule is a model for the metastable conformation of a long polymer after initial immersion in a poor solvent. Recent experimental findings describing the conformation of the human genome at the megabase scale are consistent with a fractal globule conformation. Here, we simulate the collapse of a polymer in a poor solvent using both molecular dynamics and Monte-Carlo simulations. We show that the statistics of the resulting configuration, such as radius of gyration, end-to-end distance, and contact probability, are independent of the approach used to simulate the condensation process. (* contributed equally).

¹This work is supported by NIH Grants 1P50HG006193-01 (Center for Cell Circuits) and 1DP2OD008540-01 (NIH New Innovator Award).

Leon Furchtgott
Harvard University

Date submitted: 11 Nov 2011

Electronic form version 1.4