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Fractal Globule as a model of DNA folding in eukaryotes MAKSIM IMAKAEV, LEONID MIRNY, Massachusetts Institute of Technology — A recent study (Lieberman-Aiden et al., Science, 2009) observed that the structure of the genome, on the scale of a few megabases, is consistent with a fractal globule. The fractal globule is a quasi-equilibrium state of a polymer after a rapid collapse. First proposed theoretically in 1988, this structure had never been simulated. Fractal globule was seen as a state, in which each subchain is compact, and doesn't mix with other subchains due to their mutual unentanglement (topological constraints). We use GPU-assisted dynamics to create fractal globules of different sizes and observe their dynamics. Our simulations confirm that a polymer after rapid collapse has compact subchains. We measure the scaling of looping probability of a subchain with it's length, and observe the remarkably robust inverse proportionality. Dynamic simulation of the equilibration of this state show that it exhibits Rose type subdiffusion. Due to diffusion, fractal globule quickly degrades to a quasi-equilibrium state, in which subchains of a polymer are mixed, but topologically unentangled. We propose that separation of spatial and topological equilibration of a polymer chain might have implications in different fields of physics.

> Maksim Imakaev Massachusetts Institute of Technology

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