Kinetic Walks and Compact Polymer Conformations

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Abstract:

I shall talk about self avoiding walks (SAW) that model polymer conformations. The athermal SAW becomes thermal, when we introduce non-bonded nearest neighbour contact interactions. We call this an Interacting Self Avoiding Walk(ISAW). Employing blind ant algorithms we can generate an ensemble of polymer conformations. By attaching Boltzmann weights we can calculate canonical ensemble averages of desired properties.

We can think of myopic ant algorithms that reduce attrition; but then we have to carry extra weights, called Rosenbuth-Rosenbluth(RR) weights to get averages right. These RR weights fluctuate and PERM algorithms address the problems that arise from these fluctuations.

We can interpret a myopic ant as generating Kinetic Growth Walk (KGW) - a walk that grows faster than it equilibrates. In this talk I shall consider a variant Interacting Growth Walk (IGW) that helps generate compact conformations useful in the study of low temperature behaviour of linear homopolymer. I shall also talk of calculating the entropy of Interacting Self Avoiding Walks from growth models.