P.39 The tube axis and entanglements in polymer melts

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Although the tube theory is very popular and successful, the tube concept remains evasive and ill defined. In the first part of this talk I'll describe a simple computer algorithm to construct the tube axis as a center line of the cloud of chain configurations at different moments of time. We test this algorithm on trajectories generated from simulations of concatenated well entangled ring polymers, thus avoiding all disentanglement processes. We find that entanglements are clearly manifested through the curvature of tube axis, and we can succesfully identify binary and ternary entanglements in molecular dynamics simulations. Several quantitative characteristics of entanglements are reported and discussed. The second part of this talk will discuss a definition of entanglements as persistent contacts between the mean paths of polymer chains. This definition will be tested in molecular dynamics simulation of linear melts. We trace the dynamics of individual entanglements and study their lifetime, distribution along the chain and the way they are created or destroyed.