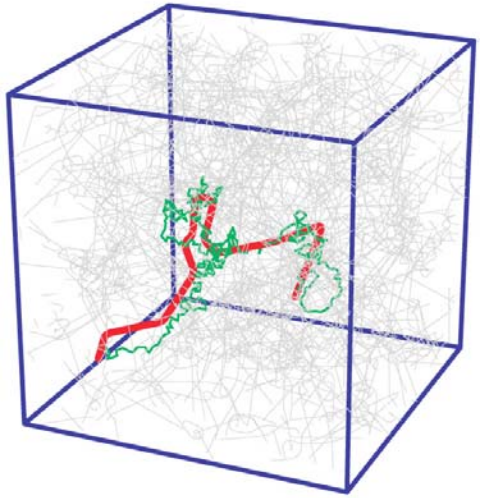
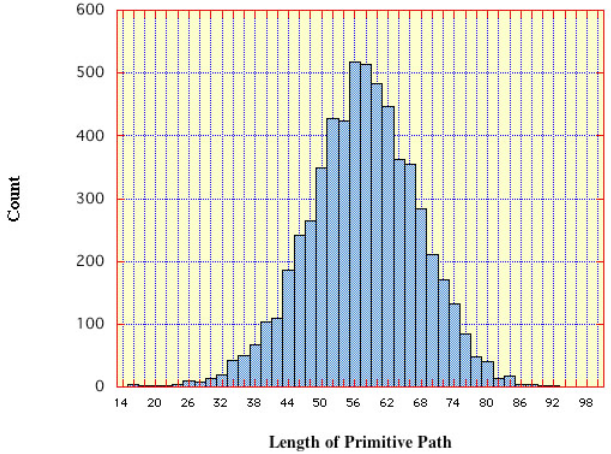
Dynamics of entangled polymers

Ronald G. Larson, University of Michigan, DMR-0305437

The viscous and elastic properties of polymers melts of interest to industry are related to the entanglements of polymer molecules with each other. As in a tangle of strings, motion of an entangled polymer molecule is restricted to directions that do not require it to cut through another polymer molecule. This restricted motion is called “reptation,” because of its similarity to the motion of a snake along its own contour. For a polymer this motion in a restricted region of space called a “tube” which follows the polymer molecule’s contour, but smooths out the fine-scale wrinkles of the real chain, as shown in the figure to the right. Although the tube is a very important concept, it has not very well defined until now. Using molecular dynamics (MD) simulations, we are now computing the distribution of tube lengths in a polymer melt, and using this to tell us about motion of both linear polymers, and those with long side branches.



A polymer chain (Green) and its corresponding axis of the tube (Red) from MD simulation.



Statistical distribution of the lengths of the tubes from MD simulations.

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Education, Outreach, and Publicity

A postdoc (Dr. Seung Joon Park), three graduate students (Sachin Shanbhag,Youngsuk Heo and Qiang Zhou) and an undergraduate student (Chris Rentsch) have been part of this work. Grad student Shanbhag had the opportunity to visit and work with the Doi Research group at Nagoya University, Japan in 2002. Prof. Doi is the world's leader on the "tube theory, and working with him has greatly helped our progress. Ronald Larson, has presented work from this grant at major invited talks at the American Physical Society, the conference on "Slow Dynamics" in Sendai, Japan, the ACS Conference on Branched Polymers in Williamsburg, Virginia, and at the Society of Rheology meeting in Minneapolis, Minnesota. Work under this grant has led to the creation of a software package that is being used at Dow Chemical Company. Portions of the work are contained in a book, "Molecular Structure and Rheology of Molten Polymers," by John Dealy and Ronald Larson. The book, currently nearing completion, is targeted towards industrial polymer scientists.