Modeling the Crystallization of Branched Polymers from Solutions and Melts

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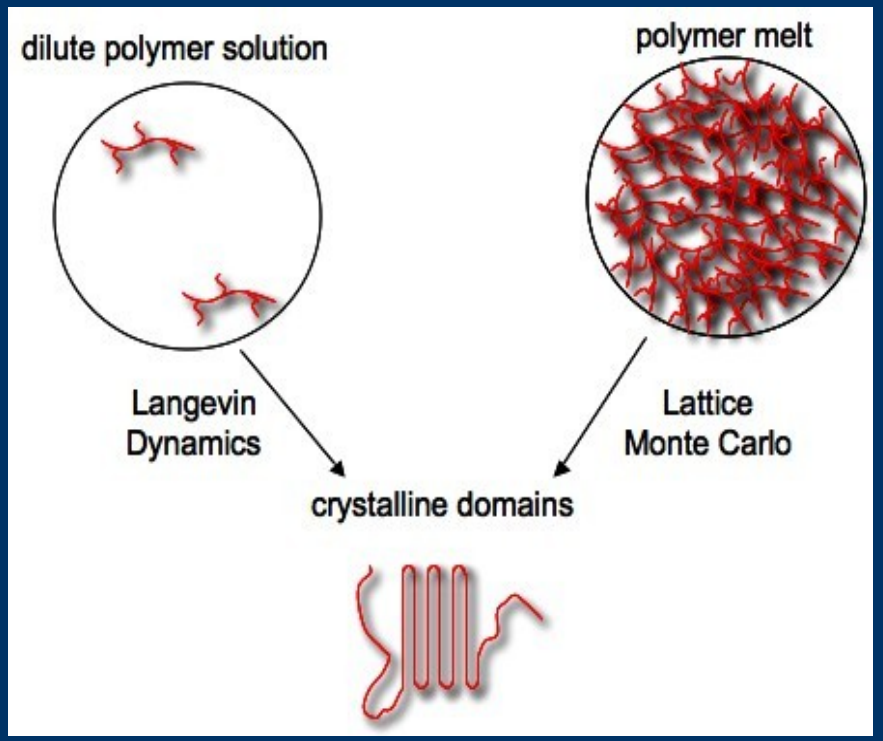
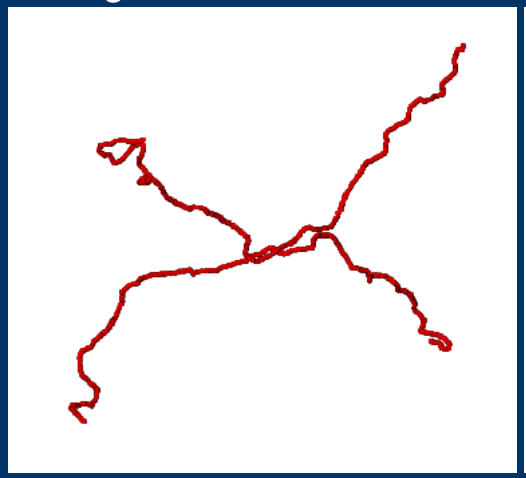
The goal of this study was to understand the nucleation of crystalline domains in linear and branched polymers, using simulations.



A Langevin dynamics, and a kinetic Monte Carlo simulation code for modeling the dynamics of polymers in solutions, and melts, respectively have been developed. Preliminary data was generated.



Based on partial analysis of preliminary data, a widespread error in the experimental literature in accounting for the driving force for nucleation at large undercoolings was spotted and communicated (Shanbhag and Alamo, Polymer, 2008).