Title: Exploring the Constraints for Random Macromolecular Configuration in Space

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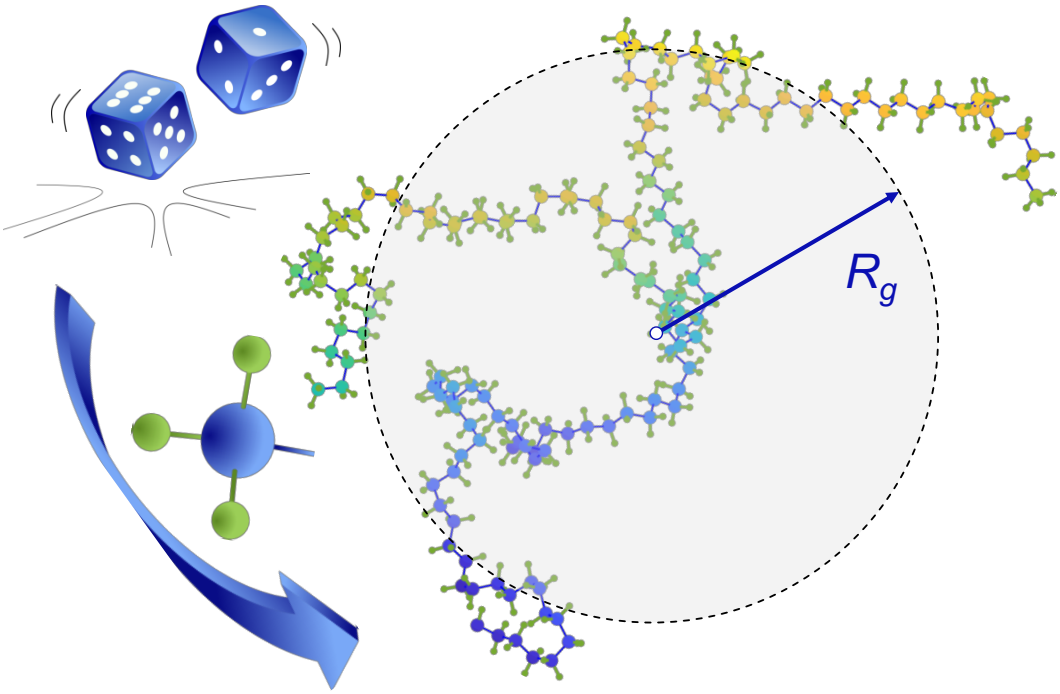
References:

Reference 1: P. J. Flory, *Principles of Polymer Chemistry*, Cornell University Press,Ithaca, NY 1953.
Reference 2: P. J. Flory, *Statistical Mechanics of Chain Molecules*, Hanser Publishers, Munich 1989.
Reference 3: V. Touloupidis, A. Albrecht, *Macromol. React. Eng.* 2022, 16, 2200002.

Images:



Abstract:

In this work, the development of a self-avoiding Monte-Carlo off-lattice three-dimensional random walk model (taking into account the bond length, the carbon-carbon angle, and steric interferences) is presented. The methodology follows the theoretical framework proposed by the pioneering work of P. J. Flory. The Monte-Carlo model developed is being validated based on experimental results of radius of gyration coming from linear polyethylene characterization by size exclusion chromatography multiangle light scattering (SEC-MALS) technique. The most detailed version of the model manages to reach an accuracy level of 80% with regard to radius of gyration, without any tuning procedure involved. Furthermore, considering the solvent effect, the accuracy level reaches a value of 95%. On the contrary, it is shown that the simplest Monte Carlo random walk model version (including only the bond length restriction) is not able to quantitatively predict the experimentally acquired values of radius of gyration. Moreover, the developed Monte Carlo model is further employed to predict the expected radius of gyration values of more complex branched topologies, demonstrating the potential of this work.