An Open-Source Python-Rust Framework for Monte Carlo Simulation of Linear and Branched Polymer Structures with Computation of Structural Descriptors

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An open-source framework has been developed for the simulation of polymer chain configurations using a Monte Carlo random walk approach, implemented through the integration of Python and Rust. The implementation is influenced by the work of Touloupidis and Albrecht. [1] Linear and branched polymer structures are generated in three-dimensional space, and realistic molecular geometries are preserved by enforcing fixed bond angles and lengths. Steric hindrance is addressed by applying spatial constraints and performing collision detection using spatial hashing techniques. Polymer topologies are represented as graph structures, enabling efficient handling of connectivity and branching. Following chain generation, structural descriptors are calculated to characterize spatial configurations. Through the combination of Rust's computational performance and Python's flexibility, scalable simulations are facilitated and integration into broader computational workflows is streamlined. This tool is intended to support research into polymer structure and the development of structure-property relationships in polymer science.

Keywords: Monte Carlo, polymer chain simulation

References

[1] V. Touloupidis, A. Albrecht, Development of a Monte Carlo Random Walk Model for the Prediction of Linear and Branched Polymer Configuration and Connection to Radius of Gyration and GPC-MALS Experimental Results, Macromolecular Reaction Engineering 16 **2022**. https://doi.org/10.1002/mren.202200002.