Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

Automated Coarse-Graining of Polyethylenimine for Simulation in Biomedicine

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ABSTRACT

Polyethylenimine (PEI) is a versatile polymer with applications in various fields of research such as gene therapy, bio-sensing, and fuel cells. Understanding the structure-function relationship of PEI is crucial for achieving the desired performance of this polymer. Synthesized PEIs are polydisperse, containing a wide range of branched structures and molecular weights. They also exhibit different protonation ratios as the environmental pH changes. Because of such variations, uncovering the structure-function relationship of individual PEIs is difficult using experimental analysis. Molecular dynamics (MD) is a useful tool that complements experimental studies by allowing the investigation of individual PEIs with well-defined structures. In this regard, several all-atom (AA) forcefields for PEI have been developed from first principles, but AA models only allow the study of small PEIs. Simulation of large PEIs can be achieved using coarse-grained (CG) models, while manual parameterization of CG forcefields is a strenuous and time-consuming task. For example, in our previous work, manually parameterization of 8 PEI structures was accomplished over a few months, which contained parameters for 98 unique bonded interactions (bond stretching, bending and torsion) accounting for merely 12% of all possible interactions.

In this work, we present a strategy that can automatically coarse-grain a large PEI molecule and generate the corresponding parameters within hours. First, the AA structure of the PEI is analyzed to determine the AA-to-CG mapping, and parameters for non-bonded interactions (van der Waals and electrostatic). Then, bonded interactions are parametrized through an iterative scheme that minimizes predefined cost functions. The strategy is implemented as a python toolbox that has been made available to the public. Validation of our methodology is demonstrated by comparing the radius of gyration and end-to-end distance of PEIs obtained from AA- and CG-MD simulations, as well as comparing the diffusion coefficient of PEIs between CG-MD simulations and experiments.

Word count: 300