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COMPUTATIONAL SOFTWARE

Polymer Chain Generation for Coarse-Grained Models Using Radical-Like Polymerization

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Abstract. This paper presents major improvements in the efficiency of the so-called Radical-Like Polymerization (RLP) algorithm proposed in "Polymer chain generation for coarse-grained models using radical-like polymerization" [J. Chem. Phys. **128** (2008)]. Three enhancements are detailed in this paper: (1) the capture radius of a radical is enlarged to increase the probability of finding a neighboring monomer; (2) between each growth step, equilibration is now performed with increasing the relaxation time depending on the actual chain size; (3) the RLP algorithm is now fully parallelized and proposed as a "fix" within the "Lammps" molecular dynamics simulation suite.

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Key words: Molecular dynamics (MD), coarse grained polymer model, LAMMPS, polymer, parallel computing.

Program Summary

Program title: Fix_rlp

Nature of problem: Implementing special fix file in parallelized LAMMPS code in order to create polymer system with the so-called Radical-Like Polymerization (RLP) algorithm proposed in [1] for coarse-grained models.

Software licence: GPL 2.0 GNU's GPL

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CiCP scientific software URL: http://michel.perez.net.free.fr/fix_rlp.zip.

Distribution format: .zip

Programming language(s): C++/MPI

Computer platform: Should run on any architecture providing a C++ compiler

Operating system: Linux or any other OS with C++ compiler and MPI library.

Compilers: C++ compiler

RAM: Depends on system size and how many CPUs are used

External routines/libraries: LAMMPS (http://lammps.sandia.gov/), FFTW (http://www.fftw.org/)

Running time: Seconds to weeks, depending on system size, speed of CPU and how many CPUs are used.

Restrictions: The code is based on a former version of LAMMPS.

Additional Comments: With the Fix_rlp LAMMPS program, you will find in the .zip detailed explanations in the"fix_rlp.txt" file, a "README.txt" file for the installation and a complete example of homopolymer generation with RLP algorithm in the form of a Lammps input file.

1 Introduction

Coarse-grained molecular dynamics is a well-adapted tool for studying the mechanical behavior of polymers [1, 2]. It is widely used for studying various mechanical properties (elastic constants [3, 4], strain hardening [5], failure [6, 7], *etc.*) for various polymer structures (linear chains [8, 9], cross-linked chains [10], branched polymers [11, 12], co-polymers [13, 14], gels [15]). To create these structures, several methods have been developed. Equilibration of fully independent self-avoiding chains [16] is a rather simple method but requires equilibration times that are not tractable with long chains. The classical "push-off" method generates self equilibrated chains by Monte-Carlo scheme (random-walk). However, long equilibration times are required to relax overlapping particles [8]. This method has been improved by introducing soft potentials [17, 18]. The equilibration stage can itself be accelerated *via* the double-bringing method [17, 19–21] or by reducing the weak interaction cut-off at the beginning of this stage [22]. They are compatible with most creation methods since they act only on equilibration, yet they don't accelerate polymer creation stage. Another method to accelerate the equilibration *via* a hybrid MD/continuum model was proposed in two versions by Kroger [23] and by Senda *et al.* [24], but is limited to rather short chains. Other kinds of methods propose simultaneous chain growth and equilibration. Subramanian recently submitted an original method where polymer chains are progressively extended by adding additional beads between two existing structural units [12, 25]. Fast algorithms, based on independent generation of chains and application of "slow push-off" potential (see *e.g.* [11]) lead