Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

A parallel algorithm to create long polymer chains in molecular dynamics[1] NICOLAS PINEAU, CLAIRE LEMARCHAND, DAVID BOUSQUET, CEA/DAM/DIF, BENOIT SCHNELL, Michelin — Generating initial configurations of polymer melts above the entanglement molecular weight is a challenge in molecular dynamics and Monte Carlo simulations. In this presentation, we describe an algorithm mimicking a chemical polymerization adapted to all-atom force fields. The principle of this algorithm is to start from a bath of monomers between which bonds are created and relaxed sequentially. Our implementation is parallel and efficient. The parallelization is that of a classical molecular dynamics code and enables the user to generate large systems, up to 7 million atoms. The efficiency of the algorithm comes from the linear scaling between the simulation time and the chain length in the limit of very long chains. The implementation is able to produce long polymer chains, up to 2000 carbon atoms, with thermodynamic, global, and local structural properties in good agreement with their counterparts obtained experimentally, by other numerical algorithms, and by the Gaussian chain model. Finally, the algorithm proposed in this work is versatile in nature because the bond creation can be easily modified to create copolymers, block copolymers and mixtures of polymer melts with other material.

[1]Fundings from the PIA project SMICE (Simulation de Matériaux pour lIndustrie par Calcul Exaflop)

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Date submitted: 19 Mar 2019 Electronic form version 1.4