Dynamical Monte-Carlo simulation of polymers in confined space: Implementation of a new algorithm

Description: Polymers confined in space are present in many real-life applications: Compacted DNA, thin layers, physics of dielectrics among others. The conformation of such polymers leads to a competition between imposed external geometry and internal arrangement of the monomers composing the polymer. The complexity of these arrangement naturally lead to the use of computer simulations of these systems in the field of statistical physics of polymers.
Among the family of Monte-Carlo simulations, two types of algorithms exist:

The statical approach consists of sequentially adding a monomer to the polymer chain in a random direction, rejecting the chains which violate compatibility with the general chain (no monomer overlap, chain inside the geometry domain) until a given number of polymers of N monomers are generated.

The dynamical method starts with a chain of N monomers, and stochastically moves a randomly chosen monomer in a random direction, then again checking if the new conformation is compatible with the internal and external constraints until a given number of polymer conformations are generated.

As the number of monomers is increased, and the confined space decreased, the dynamical method tends to reject more and more conformations mainly due to a conflict with the confined geometry.

In this project, a new dynamical algorithm is implemented in which the number of these rejections should be decreased while generating conformations. The goal of this project is to implement this algorithm, validate it agains theoretical (end-to-end distance and gyration radius, auto-correlation function,...) and other numerical methods, and benchmark its performance.

Computational Aspects:
- Algorithms
- Parallel computing (MPI)
- Scientific software design

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