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A topology user package for LAMMPS

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Abstract

We created an extension of LAMMPS, a popular molecular dynamics simulator. Our extension is a part of the creation of a larger user-package that enables the measurement of topological entanglement through rigorous mathematical measures from topology. In this part of the user-package we created a method to measure the linking in a system of macromolecules in Molecular Dynamics (MD) simulations. We present the software and explanatory material which are easily accessible to the engineering and bio-engineering community.

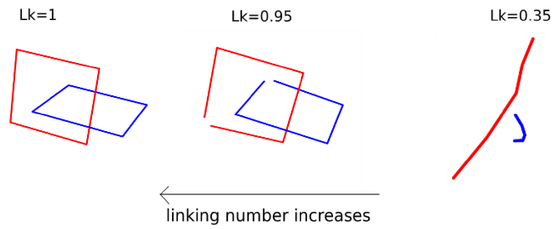
Introduction

Polymers are macromolecules that cannot cross each other without breaking their bonds. Due to this uncrossability constraint, systems of many chains impose spatial restrictions called entanglements on each other, which dramatically affect the viscoelastic properties of materials. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is a classical molecular dynamics simulation code designed to run efficiently on parallel computers and is widely used in the scientific community [2]. Measuring entanglement in such systems has been a very difficult problem partially due to the lack of rigorous measures of entanglement. In this research, we created an extension of LAMMPS which allows to measure the entanglement of polymer chains using the Gauss linking integral during a simulation. This allows scientists to use rigorous mathematical tools in simulations using LAMMPS for the first time.

Definitions

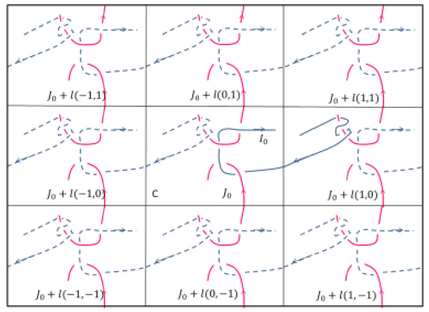
Linking Number: The Gauss linking number of two disjoint (closed or open) oriented curves l_1 and l_2, whose arc-length parametrizations are $\gamma_1(t)$ and $\gamma_2(s)$ respectively, is defined as a double integral over l_1 and l_2:

$$L(l_1, l_2) = \frac{1}{4\pi} \int_{[0,1]} \int_{[0,1]} \frac{(\dot{\gamma}_1(t), \dot{\gamma}_2(s), \gamma_1(t) - \gamma_2(s))}{|\gamma_1(t) - \gamma_2(s)|^3} dtds$$



The linking number of two curves measures how many times a curve turns around the other.
For closed chains the linking number is an integer topological invariant (it does not change as long as the chains do not cross through each other.
For open chains, the linking number is a real number that is a continuous function of the chain coordinates.

In order to avoid boundary effects, Periodic Boundary Conditions (PBC) are used in simulations. The polymeric system is created by gluing copies of the periodic box along the edges. This creates an infinite system whose periodic entanglement can be captured by the Periodic Linking Number.



Periodic Linking Number: Let I and J denote two infinite collections of chains (free chains) in a periodic system. Suppose that I_U is an image of the free chain I in the periodic system. The periodic linking number, LK_P, between two free chains I and J is defined as [1]:

$$LK_P(I, J) = \sum_{u} L(I_1, J_u)$$

Methods

The package was written in C++ in accordance with LAMMPS styling. Below is the documentation for the linking number command. It applies to ring, linear and branched polymers, in 1, 2 or 3 PBC. The options allow for the computation of the Linking Number of each pair of chains in a collection, the Periodic Linking Number, as well as the writhe and torsion (not discussed here).

compute lk command

Syntax

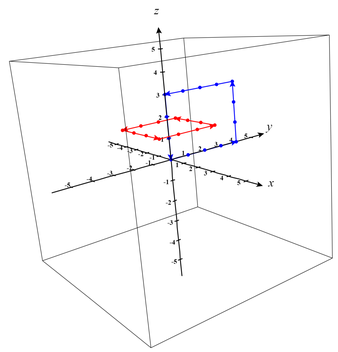
```
compute ID group-ID lk group2-ID periodicity atom-grouping
```

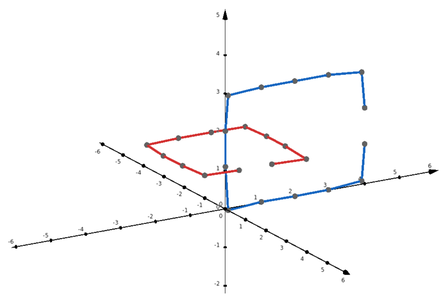
- ID, group-ID are documented in :doc:`compute <compute>` command
- lk = style name of this compute command
- group2-ID = the group-ID of the group containing the chains to be compared to those in the first group
- periodicity = the type of linking number to calculate (periodic or nonperiodic)
- atom-grouping = how the atoms are grouped (molecular if atoms have a molecule-ID, name of compute fragment command if not)

Examples

```
compute 1 all lk all periodic calcFragment
compute 2 all lk group2 nonperiodic molecular
```

Below we show how the linking number of a simple system (toy model) of two polymers varies during a simulation using a Langevin thermostat in the NVE ensemble. Left: Ring polymers, the linking number is a topological invariant, Right: Linear polymers, the linking number is a continuous function of the chain coordinates.

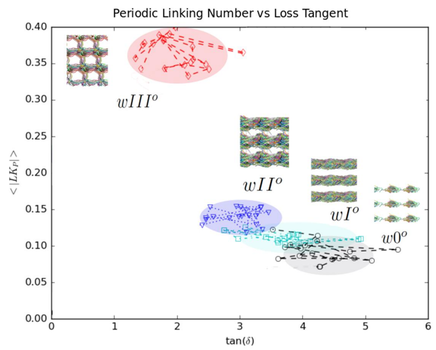




```
Step c_calcLK[1][2]
       0           -1
       5           -1
      10           -1
      15           -1
      20           -1
      25           -1
      30           -1
      35           -1
      40           -1
      45           -1
      50           -1
Loop time of 0.00256586 on 1 procs for 50 steps with 26 atoms
```

```
Step c calcLK[1][2]
       0  -0.64256727
       5  -0.64217165
      10   -0.6409973
      15  -0.63909866
      20  -0.63652578
      25   -0.6333496
      30  -0.62964963
      35  -0.62554313
      40  -0.62113047
     ...
    5000  -0.16475975
Loop time of 0.21096 on 1 procs for 5000 steps with 26 atoms
```

Applications



Initial results have shown that the Periodic Linking Number captures entanglement related to the viscoelasticity of the material [3]. Our topological user package for LAMMPS will allow for further demonstrations and more detailed analysis of the effects of entanglement in viscoelasticity in many different contexts, an open problem for more than 50 years.

References

1. Panagiotou, E. (2015). The linking number in systems with periodic boundary conditions. *Journal of Computational Physics*, *300*, 533-573.
2. Plimpton, S. (1993). Fast parallel algorithms for short-range molecular dynamics (No. SAND-91-1144). Sandia National Labs., Albuquerque, NM (United States).
3. Panagiotou E., Millett K. C. and Atzberger P., 2019, Topological Methods for Polymeric Materials: Characterizing the Relationship Between Polymer Entanglement and Viscoelasticity, *Polymers* ,11(3), 437.

Acknowledgements

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