1161-70-281   **Tom Herschberg*** (`mgr992@mocs.utc.edu`) and **Eleni Panagiotou**. *A Topology User Package for LAMMPS.*

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. (Received August 18, 2020)

1