Tutorial

10: MD Simulation of Polymers/polyelectrolyte with ESPResSo

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In the tutorial we want to simulate a single polymer/polyelectrolyte chain in an NVT ensemble with ESPResSo.

1 Tasks

1. Check the code tutorial_single_chain.tcl to find how to to simulate one neutral polymer chain, and how to simulate one polyelectrolyte with counterions.
2. Use VMD to look at the trajectory of the MD simulations.
3. Change the chain length to find the relation between the chain length and the radius of gyration.

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