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MS 58 – Young Investigators Minisymposium: The Influence of the Lennard-Jones-Potential in Steered Molecular Dynamics Tensile Test Simulations

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(2) Presentation of things that did not work (as expected)
In our simulations, we perform tensile tests on bundles of peptides using Coarse-grained Steered Molecular Dynamics in *LAMMPS* [1]. The original peptide molecules are modeled as strings of "beads", where the force-field between the beads represents the mechanical behaviour of the peptide molecules in full-scale atomistic simulation. The respective parameters were obtained from a previous study by *Depalle et al.* [2]. Between the strings we insert cross-links with relatively low strength.
In order to capture the failure of the bonds with a reasonable timestep, we used a regularisation approach, where the force between two particles is not eliminated directly after having reached the critical distance of bond rupture, but is smoothed out. This was applied for bonds within the bead strings and cross-links.
Nevertheless, we still were facing problems when performing our tensile tests - simulations were not running. We could see that single beads were experiencing high forces just before rupture, but were only concentrating on force-field we had defined for the bonds, when searching for the reason that caused this problem.
In the end, it turned out that the reason was not the definition of the bonds, but the Lennard-Jones (LJ) Potential we naturally applied. The breaking bonds were only the original reason, causing a kind of chain effect were beads would penetrate each other, leading to high forces between two particles due to the high gradient of the LJ Potential in the repulsive zone. The timestep was not small enough to capture these effects, but particles were "shot out" of the simulation box. A soft core was added to the LJ-Potential and could finally solve the problem.

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