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Multi-scale modelling and dynamics

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Moving from a fine-grained particle model to one of lower resolution leads, with few exceptions, to an acceleration of molecular mobility, higher diffusion coefficient, lower viscosities and more. On top of that, the level of acceleration is often different for different dynamical processes as well as for different state points. While the reasons are often understood, the fact that coarse-graining almost necessarily introduces unpredictable acceleration of the molecular dynamics severely limits its usefulness as a predictive tool. There are several attempts under way to remedy these shortcoming of coarse-grained models. On the one hand, we follow bottom-up approaches. They attempt already when the coarse-graining scheme is conceived to estimate their impact on the dynamics. This is done by excess-entropy scaling. On the other hand, we also pursue a top-down development. Here we start with a very coarse-grained model (dissipative particle dynamics) which in its native form produces qualitatively wrong polymer dynamics, as its molecules cannot entangle. This model is modified by additional temporary bonds, so-called slip springs, to repair this defect. As a result, polymer melts and solutions described by the slip-spring DPD model show correct dynamical behaviour. Read more: "Excess entropy scaling for the segmental and global dynamics of polyethylene melts", E. Voyiatzis, F. Müller-Plathe, and M.C. Böhm, Phys. Chem. Chem. Phys. **16**, 24301–24311 (2014). [DOI: 10.1039/C4CP03559C] "Recovering the Reptation Dynamics of Polymer Melts in Dissipative Particle Dynamics Simulations via Slip-Springs", M. Langeloth, Y. Masubuchi, M. C. Böhm, and F. Müller-Plathe, J. Chem. Phys. **138**, 104907 (2013). [DOI: 10.1063/1.4794156].