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Coarse-graining and dynamics of complex macromolecular liquids: melts and blends MARINA GUENZA, University of Oregon — Processes of scientific interest in macromolecular liquids can involve more than ten orders of magnitude in space and time variables, impairing our ability of performing atomic-level simulations in the long-time regime. A way to overcome this problem is to resort to multiscale modeling procedures. Here the challenge is to have a formally rigorous, possible analytical, coarse-graining procedure that enables accurate transfer of information between different lengthscales of interest. Starting from the Ornstein-Zernike equation we derived (G.Yatsenko et al. PRL 93, 257803 (2004)) an analytical procedure to coarse-grain structure and dynamics of macromolecular liquids (homo- and diblockco-polymers) and their mixtures. Our procedure maps macromolecules into interacting soft-colloidal particles and provides the effective soft-core potentials input to mesoscale simulations of the coarse-grained systems. Because analytical, our procedure provides a universal formalism easily implemented to treat different systems of interest. Our procedure efficiently extends the range of length- and timescales accessible in simulations of macromolecular liquids. The soft-core mean-force potential enters the Langevin Equation for Cooperative Dynamics (M.Guenza PRL 88, 025901 (2002)), which predicts anomalous subdiffusive center-of-mass motion in excellent agreement with simulations and recent experimental data.

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