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New perspectives for molecular field simulations of complex fluids

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Molecular field simulations have been introduced a while ago as a dynamic extension of the self-consistent field theory, one of the most successful theories for the description of inhomogeneous polymer systems. They build on a continuous free energy functional, which however incorporates details on the structure and architecture of the molecules. In that sense, they bridge between particle-based simulations of complex matter and continuuous simulations based on phase field theories such as the Cahn-Hilliard theory. In the talk I will first very briefly review the basic concept of molecular field simulations, and then present three recent extensions developed in our group. (i) A method to introduce hydrodynamic interactions by coupling molecular fields to a Lattice-Boltzmann fluid model; (ii) A method to deal with permanent crosslinks, i.e., to deal with polymer networks; and (iii) An approach to couple molecular field simulations with particle-based simulations in an adaptive multiscale scheme.

[1] L. Zhang, A. Sevink, F. Schmid, Macromolecules 44, 9434 (2011).
[2] F. Schmid, Phys. Rev. Lett. 111, 028303 (2013).
[3] S. Qi, H. Behringer, F. Schmid, New J. Physics, accepted (2013).