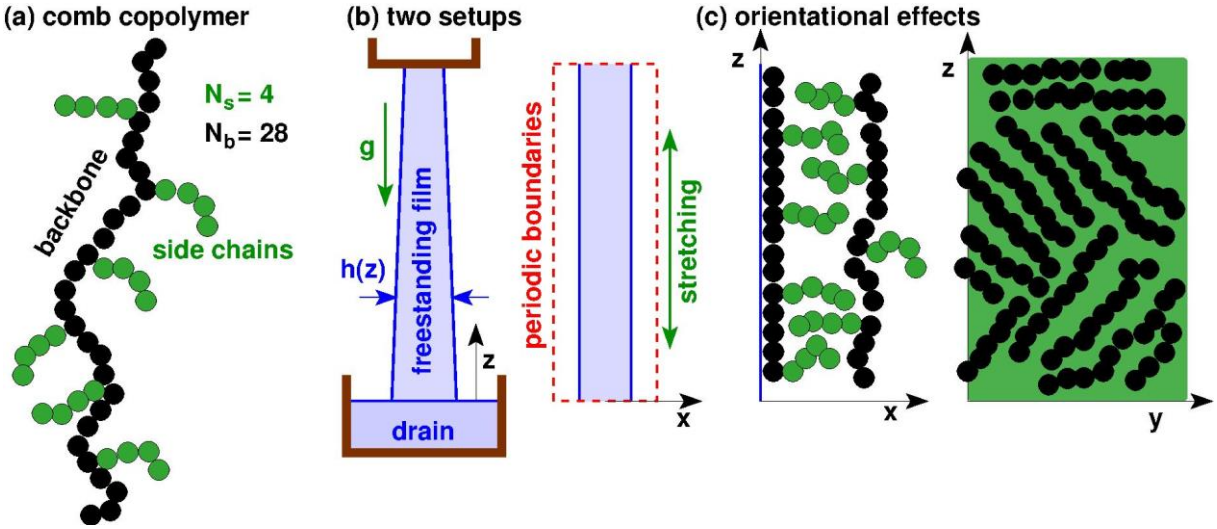
Molecular dynamics simulation of comb copolymer films

DIRECTEUR DE THESE : JOACHIM WITTMER
INSTITUT CHARLES SADRON, 23, RUE DU LOESS, 67034 STRASBOURG
TEL : 03 88 40 41 55; E-MAIL : JOACHIM.WITTMER@ICS-CNRS.UNISTRA.FR

Freestanding thin films of comb copolymer melts far above the glass transition have been shown experimentally to be stable for more than a day [1]. This is several orders of magnitude longer than expected from the rheological properties of the bulk phase. To understand this striking observation we propose to investigate conformational and rheological properties of such films by means of molecular dynamics simulations of a coarse-grained polymer bead-spring model. Different possible scenarios will be addressed by tuning the model Hamiltonian and the film preparation history closely comparing our numerical approach with the experimental results obtained in the new research group of W. Drenckhan at the ICS. This complementary study may lead ultimately to new developments in polymeric thin films, foams and emulsions without the use of stabilizing agents opening new perspectives in fields such as cosmetics and material design [1].



Sketch of problem addressed: **(a)** Coarsed-grained comb copolymer model with a long backbone chain. We assume that all (sub)chains are monodisperse and that the side chains are fixed at constant intervals along the backbone. **(b)** Drainage under gravity (left) and film stretching using the periodic boundary conditions (right). The width h of the film is (on average) constant in the second setup. **(c)** Orientational ordering perpendicular (left) and parallel (right) to one of the film interfaces. Only the backbone monomers are drawn in the second case.

The proprosed project is ideally suited for a PhD thesis.

[1] T. Gaillard, C. Poulard, T. Voisin, C. Honorez, P. Davidson, W. Drenckhan, M. Roche, Macro Letters, Stable freestanding thin films of copolymer melts far from the glass transition, **4**, 1144 (2015)