Wang-Landau Monte Carlo simulations of single ABC miktoarm star block copolymers (M.Sc./speciale)

The behavior of single polymer chains under different solvent conditions plays a central role in polymer physics. This is also the case when different chains are combined to form block copolymers (see Fig.(a)). A single homopolymer chain in a so-called bad solvent will collapse to a structureless compact globule minimizing unfavorable contact between the solvent and the monomers. Introducing two kinds of monomers A and B immediately gives rise to a much richer behavior. In particular, micro-phase separation is possible, leading to various interesting internal structures (Fig. (c)). In this project you will use a Wang-Landau Monte Carlo simulation setup developed by Drew Parsons in Perth to investigate 3-armed ABC star molecules (see Fig.(b)). The major interest is how confinement within a globule, which in this case is a flexible kind of confinement, affects the resulting morphology. In Fig.(c) results from 2 component AB diblocks are shown.

Figure: (a) An AB diblock copolymer (b) An ABC miktoarm terpolymer. (c) Single chain structures formed by a AB_n diblocks (a chain of AB's) in poor solvent for both blocks A and B.

The project will be remotely co-supervised by Drew Parsons who is supplying the basic C++ code to be modified and expanded by you in this study.

Prerequisites:

- ✓ Coding experience - not so important in what language but C++ of course an advantage.

As a student you will:

- ✓ get an understanding of the fundamentals of Wang-Landau Monte Carlo simulations.
- ✓ perform simulations independently
- ✓ learn about polymer physics/chemistry
- ✓ learn about complex self-assembly

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Reference:
Parsons and Williams, Phys. Rev. Lett., 99, 228302, 2007