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. 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.(a)). 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.(b) 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 ABₙ 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

Supervisor(s):
Jacob Kirkensgaard (jikk@nbi.dk) and Drew Parsons, Murdoch University, Perth, Australia

Reference:
**Block copolymer self-assembly under hyperbolic confinement**

Numerical simulations reveal a family of hierarchical and chiral multicontinuous network structures self-assembled from a melt blend of Y-shaped ABC and ABD three-miktoarm star terpolymers, see figure below. These mesostructures are among the most topologically complex morphologies identified to date and represent an example of hierarchical ordering within a hyperbolic pattern, a unique mode of soft-matter self-assembly. In this project the idea is to implement a simulation setup to investigate the self-assembly of model block copolymers under different hyperbolic constraints, i.e. where the polymer are forced to assemble within a thin curved film.

**Prerequisites:**

✓ Preferably coding experience - not so important in what language

**As a student you will:**

✓ get an understanding of the fundamentals of DPD and MD
✓ implement new hyperbolic constraint simulations
✓ learn about polymer physics/chemistry
✓ learn about complex self-assembly and hyperbolic geometry

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**Figure:** In blends of ABC and ABD stars (A) the green and yellow majority domains form two intertwined chiral srs nets (B) separated by a hyperbolic film made from the blue and red minority components.

**Supervisor:**
Jacob Kirkensgaard ([jjkk@nbi.dk](mailto:jjkk@nbi.dk)) [http://www.nbi.dk/~jjkk/](http://www.nbi.dk/~jjkk/)

**Reference:**
Kirkensgaard JJK, Evans, de Campo and Hyde, PNAS, 111, 4, 1271-1276 (2014)
Simulation and experimental study of block copolymers self-assembling under spherical confinement

A relatively new, but conceptually simple experimental procedure makes it possible to form spherically confined nano-particles out of block copolymers by a clever evaporation of mixed good and bad solvent for the polymers. A new simulation setup allows to simulate such spherically confined systems of arbitrary mixtures of block copolymers which reproduce existing experimental results for diblock copolymers. In this project the idea is to investigate the effect of confinement on new metal containing diblocks and/or ABC star polymeric systems which in the melt state form many complex structures already.

Prerequisites:
✓ Basic lab experience

As a student you will:
✓ prepare block copolymer nanoparticles at DTU Nanotech
✓ do simulations as in the figure using Dissipative Particle Dynamics
✓ do structural analysis of particles: scattering and electron microscopy
✓ invent new relevant computational analysis methods?
✓ learn about polymer physics/chemistry and complex self-assembly

Figure: Simulation results from spherically confined linear AB diblocks and ABC triblocks as a function of the D/L_0 ratio, where D and L_0 correspond to the particle diameter and the period of lamellar structure in the films, respectively.

Supervisor(s):
Jacob Kirkensgaard (jjkk@nbi.dk), http://www.nbi.dk/~jjkk/
External supervisor Sergey Chernyy, DTU

Reference:
Kirkensgaard, JJK, Soft Matter, 2010, DOI: 10.1039/c0sm00358a
Block copolymer self-assembly under double spherical (shell) nano-confinement

A relatively new, but conceptually simple experimental procedure makes it possible to form spherically confined nano-particles out of block copolymers by a clever evaporation of mixed good and bad solvent for the polymers. A new simulation setup allows to simulate such spherically confined systems of arbitrary mixtures of block copolymers which reproduce existing experimental results for diblock copolymers. In this project the idea is to investigate the effect of such confinement when the polymers at the same time are restricted to move on an inner sphere which could either be a metal nanoparticle or a liquid core (see reference).

If this is a Master project there is a possibility to expand the project experimentally.

As a student you will:

✓ expand a currently running simulation setup to double confinent
✓ invent new relevant computational analysis methods?
✓ learn about polymer physics/chemistry and complex self-assembly

![Figure: Liquid core nanoparticles formed from PS-PMMA diblock copolymers in hexadecane.](image)

**Supervisor(s):**
Jacob Kirkensgaard ([jjkk@nbi.dk](mailto:jjkk@nbi.dk)), http://www.nbi.dk/~jjkk/
If experimental: External supervisor Sergey Chernyy, DTU

**Reference:**
Staff *et al.*, Soft Matter, 2011, 7, 10219
Structural characterization of thylakoid membrane stacks

Thylakoid membranes (TM) are a vital part of the photosynthetic machinery in green plants, cyanobacteria and algae as most of the proteins taking part of the light capturing is embedded in this membrane system. TM’s has a very striking organization on mesoscales as they arrange into stacked cylindrical domains, ‘grana’, surrounded by membrane sheets, ‘stroma lamellae’, connecting other grana (see Figure). Ultimately we are interested in the role of this organization in the process of photosynthesis and specifically the structural behavior in the grana stack.

The project will be focused on structural characterization of well-defined TM’s cross-characterized by electron microscopy. This will be done performing detailed measurements using Small-Angle X-ray Scattering (SAXS). There are many possible directions for a project within this field - please come and discuss with the supervisors listed below.

As a student you will learn about:

✓ ultrastructure of plant organelles, membrane organization and molecular details of photosynthesis with special emphasis on bio/nano-technological applications
✓ small-angle scattering theory and applications

and you will get to:

✓ prepare samples in the photosynthesis group lab using various biochemical methods
✓ perform small-angle scattering experiments on the SAXS camera at NBI
✓ perform data analysis on the experimental data possibly complemented by theoretical model calculations using MATLAB (thus - you will learn to use MATLAB as well...)
✓ be a part of a cross-disciplinary research collaboration within KU

Supervisor(s):
Jacob Kirkensgaard (jjkk@nbi.dk) http://www.nbi.dk/~jjkk/ and Dainius Jakubauskas
External supervisor: Poul Erik Jensen (Plant Science)

Reference:

Figure: Electron microscopy image of green plant chloroplast showing the thylakoid membranes.