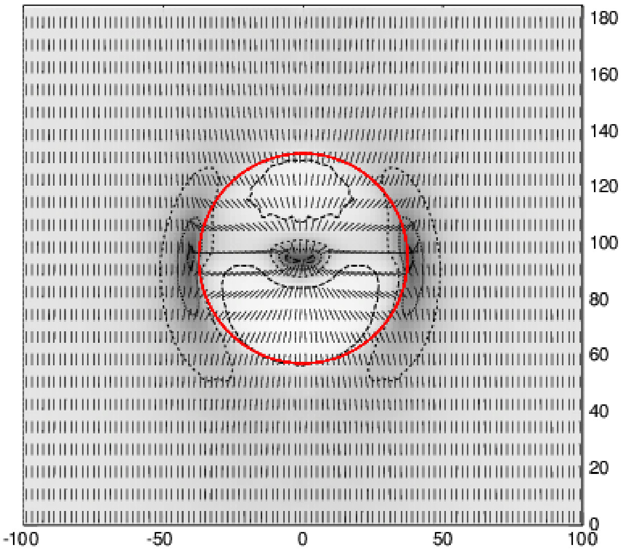
Report on PIRSES visit of O. Farenyuk, Institute for Condensed Matter Physics, NANU. (September 2012) to: UMCS, Lublin, Poland.

During this visit I was involved in two activities: (a) writing computer code to provide a way for extensive analysis of coarse-grained molecular dynamics simulations of colloid particles in a nematic solvent; and (b) performing computer simulations for the Janus particles immersed into a nematic solvent and analyzing the arising defects of the nematic director around them.

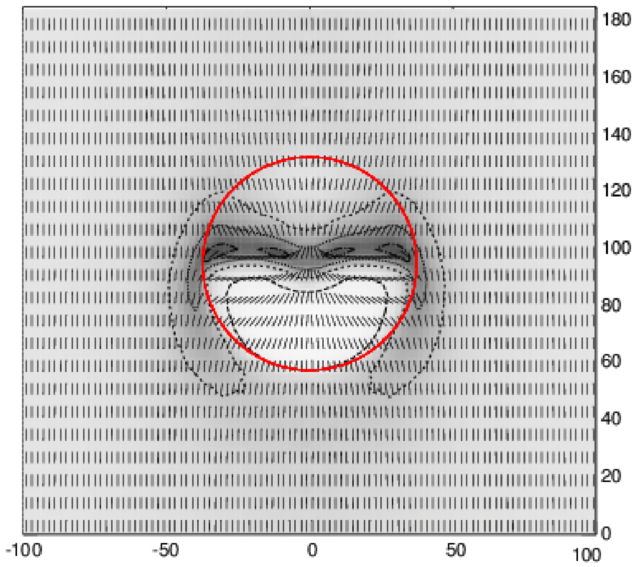
As the result of activity (a) the program code “lc_an” was written on c++ available to use for other members of the group. It reads the coordinates files obtained via (coarse-grained) molecular dynamics simulations, splits the system into cuboidal domains of desired dimensions and analyses nematic tensorial order in each domain. Then, the averaging of density, scalar nematic order and nematic director is performed over azimuthal angle to build the 2D projection of the averaged director field. The result is presented in a form of gnuplot script using a set of commands centered around the splot one. The visualization plots for the director structures in this report and in the report by J.Ilnytskyi are build using this code.

Within the activity (2), the method of coarse-grained molecular dynamics, described in more detail in the report by J.Ilnytskyi, was applied to the simulation of defects in nematic liquid crystal around the so-called Janus-particles. These are symmetric spherical particles composed of two hemispheres, each one differs by the type and/or the strength of anchoring potential. We performed simulations for different orientations of the separating plane normal vector in respect to the bulk director field. However, at this stage, the analysis is performed for one particular case only, for which the plane normal vector is collinear to director field. For other orientations further analysis need to be performed.

To build the director distribution around Janus-particle extensive simulations were performed for the case of colloid size $R=10\sigma_0$. In particular, we consider following cases: (i) non-Janus particle, with the homeotropic anchoring of equal strength on both hemispheres used as a reference system; (ii) asymmetric homeotropic-homeotropic Janus particle, with constant homeotropic anchoring on one hemisphere and reduced homeotropic constant on another hemisphere); (iii) homeotropic-planar Janus particle with the planar anchoring of various strength on one of hemispheres. It was shown that Saturn-ring defect (observed in the case (i)) remains stable, though displaced to a small distance in the direction of stronger field for the case (ii) with the homeotropic constants ratio approximately equal to or greater then 5/2 (Fig 1.a). For smaller ratios, defect transforms to the Saturn semi-ring – which exists only above surface of hemisphere with greater anchoring field (Fig 1.b). The defect diminishes when anchoring on one hemisphere vanish, but it still exists even at zero anchoring on one of hemispheres. For the case (iii) it is also present, being small for weak planar anchoring and becomes wider with the planar anchoring growth (Fig 1.c). Starting from planar anchoring force, approximately 5/2 times lower than homeotropic anchoring on opposite hemisphere, “bojoom”-like defect forms on the polar region of planar hemisphere. Further study showed that it is metastable for smaller force. Details of defects transformations require additional investigations.



a)



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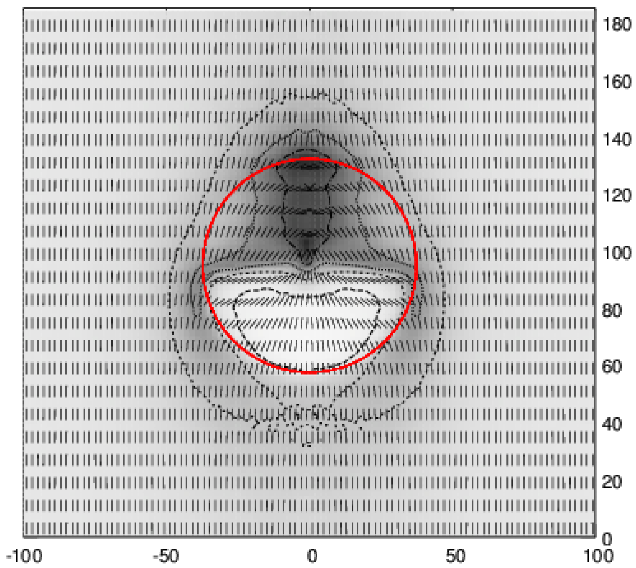

c)

Fig. 1. Director field and order parameter around colloidal particle of radius $R=10\sigma_0$. Corresponding anchoring type and effective force for upper and lower hemisphere:
a) homeotropic, 3 / homeotropic, 5
b) homeotropic, 1 / homeotropic, 5
c) planar, 3 / homeotropic, 5

This study was extended further to the case of larger colloid size, $R>15\sigma_0$. We considered only the case (iii) with the homeotropic and planar anchoring of equal strength (the same value of force constant). It was shown that both Saturn semi-ring defect and “bojoom”-like defects covers larger part of particle with the increase of colloid size, effectively surrounding it for $R=15\sigma_0$ and above (Fig 2.), this holds for the colloid sizes at least up to $R=30\sigma_0$. Behavior for larger colloid particles was not yet studied. It is important to note that formation of that cover takes time by orders of magnitude longer than equilibration on the average of the bulk.

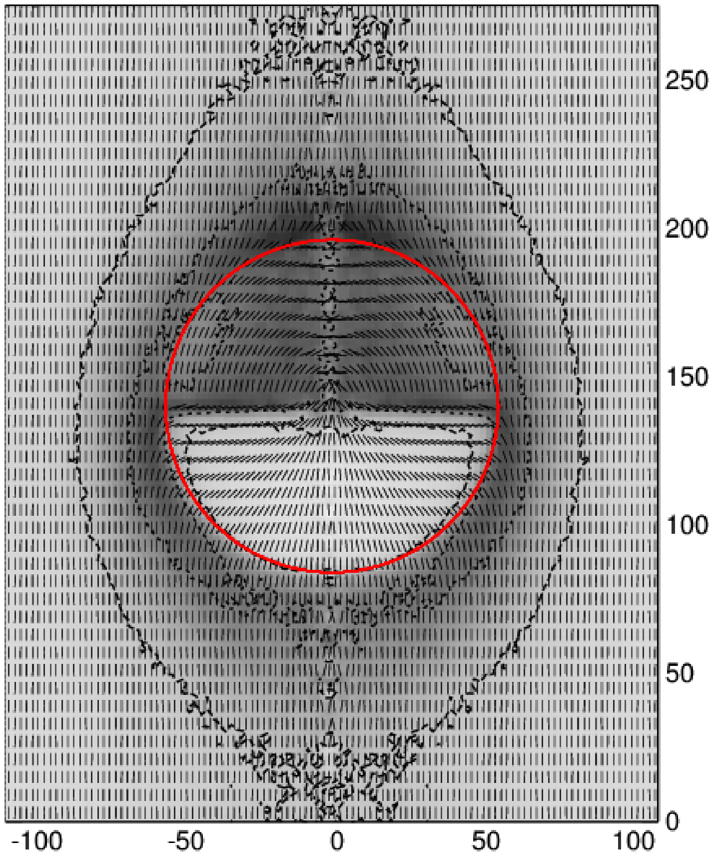

Fig. 2. Director field and order parameter around colloidal particle of radius $R=15\sigma_0$. Homeotropic anchoring on lower hemisphere, planar on upper.

The study being done provides a basis for further investigations of the behavior of Janus particles, in particular the defects arising near surfaces (which affect the symmetry of the director field) and their aggregation in bulk, due to the effective interactions of Janus particles via the deformation of director field, according to the director field around each particle studied during this scientific visit.