Report on PIRSES visits for J.Ilnytskyi, Institute for Condensed Matter Physics, NANU.
1-30 September 2012, visit to: University Maria Curie-Sklodowska, Lublin, Poland, Prof. S. Sokolowski

Scope of work: Modelling of Janus particles in the nematic solvent with the use of coarse-grained potentials, modeling of a Poiseuille flow in a microchanmnel with polymer modified walls.

The coarse grained model potential for liquid crystal particles developed by Lintuvuori and Wilson [J.S. Lintuvuori, M.R. Wilson, J. Chem. Phys. 128, 044906 (2008)] is applied for the simulations of the defects in nematic liquid crystal around spherical Janus particle. The main advantage of using these potentials is the ability to consider the systems of large sizes required in such simulations. Various types of the liquid crystal-colloid interaction were tested including the cases of a soft repulsive large sphere-spherocylinder Kihara potential, the virtual shell of spherical particles located on colloid surface, and the same shell of radially oriented spherocylindrical particles. All models mentioned above turned to be prone to essential density inhomogeneities around the surface of colloid. To avoid this artefact, we choose to model a colloid particle as a collection of the same spherocylinder particles that represent the liquid crystal around it, but the particles forming colloid have their orientation frozen by application of the external field which acts inside a sphere of the radius R. The circularly oriented field (the spherocylinders are oriented parallel to the vector running out of the colloid center) is used for representing the homeotropic anchoring, whereas the anticircular field (the spherocylinders are oriented perpendicularly to the vector running out of the colloid center) is used for the case of planar anchoring on the colloid surface. Simulations are performed using the coarse-grained molecular dynamics code developed by J.Ilnytskyi by modification of the gbmoldd package [J. Ilnytskyi, M.R. Wilson, Comput. Phys. Comm. 134, 23 (2001), ibid. 148, 43 (2002)].

The cases of uniform anchoring (both planar and homeotropic) were considered at first. In the case of planar anchoring essentially the same “bojoom”-like defect is found on both north and south caps of the colloid for all colloid sized being studied ($R=10\sigma_0$-$67\sigma_0$), where $\sigma_0$ is the diameter of the cap for the spherocylinders (see, Fig.1). The length-scale of the defect, however, depends on elastic properties of the nematic and does not scale with the increase of R.

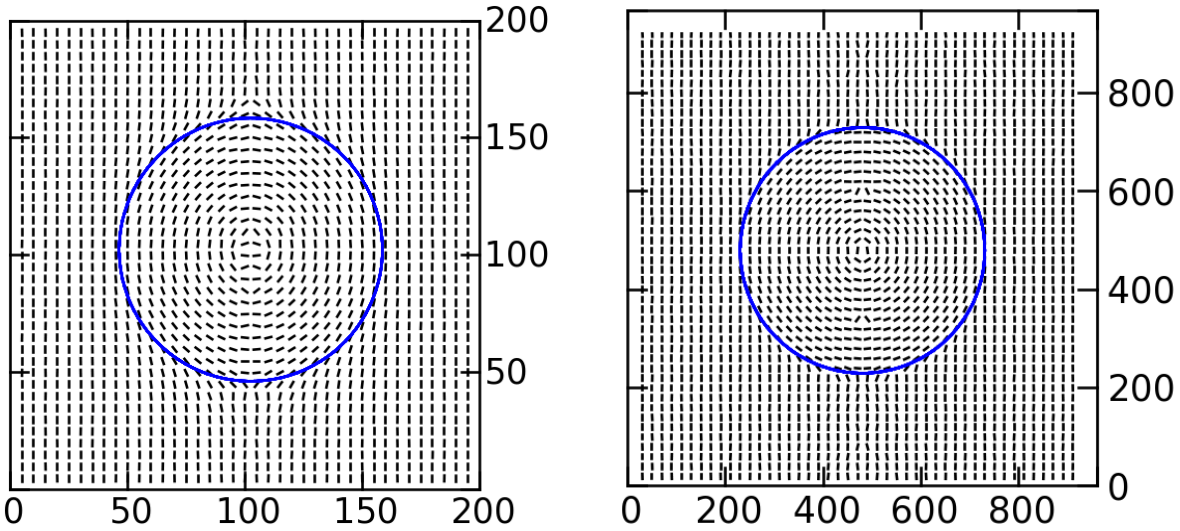


Fig.1. Director field for the “bojoom”-like defect around colloidal particle of radius $R=15\sigma_0$ (left frame) and $R=67\sigma_0$ (right frame) obtained for a planar anchoring around the colloid.

In the case of homeotropic anchoring it is predicted that for smaller R the Saturn-ring defect (of a quadrupolar symmetry) is the stable one, whereas at larger R the satellite defect (of dipolar symmetry) is more stable [H.Stark, Physics Reports 351, 387 (2001)]. Previous simulations [D. Andrienko, G. Germano, M.P. Allen, Phys.Rev. E, 041701 (2001)] used the semi-atomistic simulations with the Gay-Berne potential and were able to advance to the colloid sizes of $R=15\sigma_0$ (using 1 million liquid crystal molecules). When started from the satellite defect ansatz for the director field, the defect was found to be at least metastable for the simulation runs expoited. Within the coarse-grained model employed by us, we advanced up to the colloid sizes of $R=80.2\sigma_0$ (using up to 6.6 million coarsed-grained liquid crystal molecules). Starting from the nematic initial state, the Saturn ring effect is always found for all R. Starting from the satellite defect ansatz for the director field and given the system to relax with no external field, we found the satellite defect to split and transform slowly into off-center ring and then into a Saturn ring for colloid sizes of $R=10\sigma_0$-$40\sigma_0$ (see, Fig.2 for the case $R=26.7\sigma_0$).

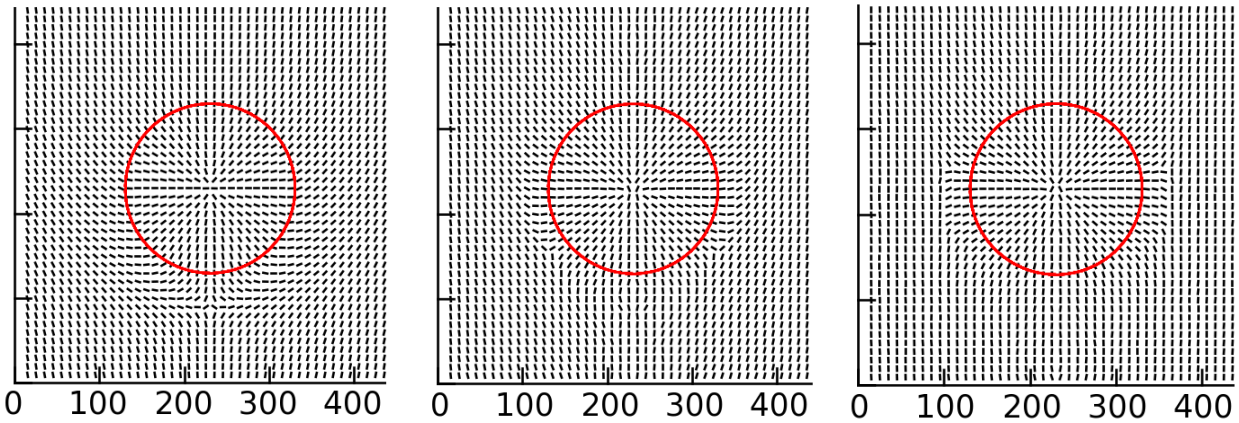


Fig.2. Transition from initial satellite ansatz for the director field (t=0, left frame) into off-center ring (t=0.8ns, middle frame) and finally into a Saturn ring defect (t=3.5ns). Colloid size: R=26.7σ0, total number of spherocylindrical particles: 347000.

For larger colloid sizes ($R>50\sigma_0$) the sattelite defect ansatz for the director stays stable for the simulation runs being performed, t=0.5ns, but given the size of the system (3.16, 3.16 and 6.6 million particles for colloid sizes of $R=53.5\sigma_0$, $R=66.8\sigma_0$, $R=80.2\sigma_0$, respectively) it should be allowed more time for the equilibration (this is especially true for the simulations without external field that are used here). The director field after the satellite defect ansatz is allowed to relax for t=0.5ns for the colloids sizes $R=53.5\sigma_0$ and $R=66.8\sigma_0$ is shown in Fig.3. The question of stability of the satellite defect for larger colloids is, therefore, still opened, and the verification of this requires these simulations to be continued at list tenfold.

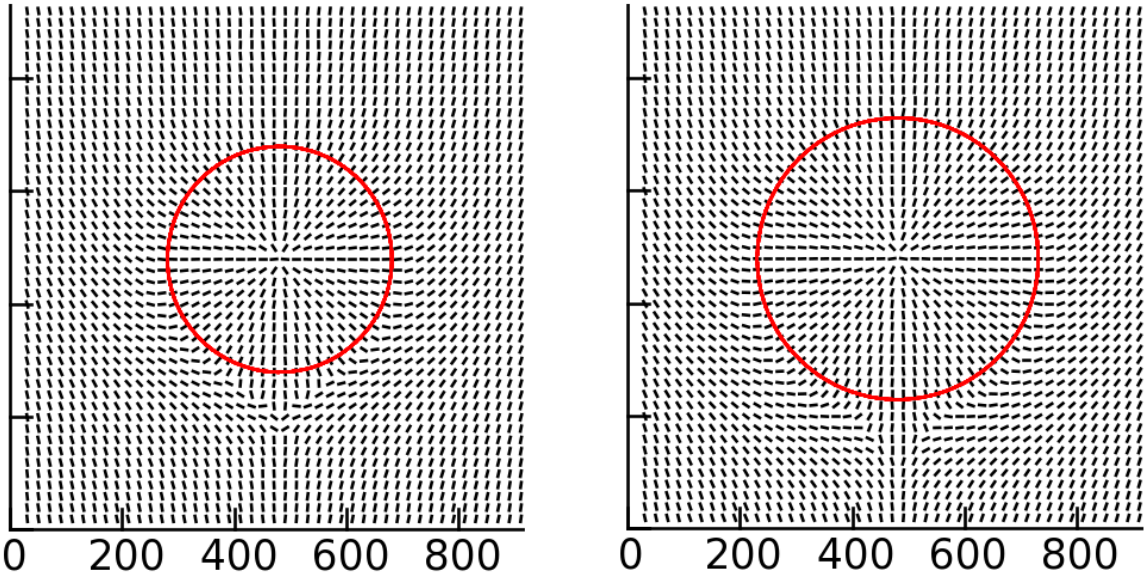

Fig.3. Director field after the initial satellite ansatz is given 0.5ns to relax for the colloid sizes of $R=53.5\sigma_0$ (left frame) and $R=66.8\sigma_0$ (right frame). Total number of spherocylindrical particles in both cases is 3.16 millions.

The simulations of the colloids with uniform anchoring undertaken during this visit prove the basis for the simulations of Janus particles, which have one semisphere with homeotropic and another – with planar anchoring. This situation is modeled via the spacially-inhomogeneous external filed applied within the sphere of radius R. The sphere is split into two semispheres with radial and antiradial symmetry of the external field (mimicking homeotropic and planar anchoring, respectively). The coarse-grained simulations of Janus particles during this visit was performed together with O.Farenyuk and are covered in his report.