Report
Andrij Trokhymchuk
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The second visit to UMCS in Lublin was dedicated to the activities set within the task **T3.3. Towards realistic models of self-assembled phases formed by complex organic fluids.**

Studies of dense solutions and melts of spherical particles grafted with fixed number of polymer chains can be performed applying the microscopic polymer reference interaction site model (PRISM) integral equations, similar to those developed by Jayaraman and Schweizer [A. Jayaraman and K.S.Schweizer, *Macromolecules,* **41**, 9430 (2008)]

Our final goal is to write down the PRISM/RISM code for the three-component system where species a = polymer tethered to colloid, species b = **colloid** and species c = **fluid** which can either molecular fluid or polymer. However, during this visit we were working to write down the PRISM/RISM code for the two-component system only, namely, the spheres in a polymer solution (polymer melt).

The PRISM/RISM code that we developed is composed of the following most important files:

Filename.h only has variable name declaration
Filename.c is the code file written in C
Input.txt is the inputfile.
PRISM.Main.c is the main code that has the main flow of all information
PRISM.Omega.c contains all the information on the intamolecular structure wij(k) molecules - i.e. the shape of the molecule. This is where we distinguish between spherical particle and polymer chain.
PRISM.Potential.c contains the information on potentials
PRISM.Structure.c calculates the structure factors Sij(k).

There are other files which are not so important.These includes:

PRISM.Picard.c that has information on the picard iteration
PRISM.Output.c deals with how to print the output files
PRISM.sinft.c deals with fourier transform stuff
PRISM.Subsystems.c describes vector, matrix arrays, used through out the code

As a test we have applied this code to calculate the effective interaction between two spheres immersed into a polymer environment – polymer suspension. The effective interaction is defined by the local structuring of the polymer chains in the vicinity of the spheres. For their theoretical determination, a full knowledge of the microscopic structure of the polymer medium is needed. The description of this structure in a uniform fluid is provided by the radial distribution functions *g(r)* or, correspondingly, the total correlation functions *h(r) = g(r)-1*. We have employed the PRISM approach to determine these functions. Then the effective interaction between diluted spheres can be identified with the potential of mean force, *w(r) = -kT*ln *g(r)*. Two cases for polymer suspension has been considered – rigid chains and flexible chains. Size ratio of the particle diameter to polymer segment diameter was fixed at 5:1. The figure shows respective radial distribution function of the particles diluted in polymer suspension of packing fraction 40%.