Polymeric materials with complex molecular architecture find numerous applications in advanced technologies, particularly in coatings, dispersants, biomedical and cosmetic materials (like drug carriers). Therefore, the synthesis of copolymers, stars, dendritic macromolecules, gels, micro- and nanogels with precisely controlled structure and properties is of the great importance. The theoretical studies of the polymerization of these systems and the prediction of structures are very difficult. It is even more complicated when macromolecules with complex internal architecture are obtained under the polymerization process with changing conditions, like medium viscosity, during the reaction. Computer simulations can provide valuable in such cases. The development and verification of the simulation methods suitable for a particular polymerization method should make possible the estimation of the optimal reaction parameters to obtain product of desired structure and properties. It will save the experimental work time and lower the cost of chemicals needed to perform the laboratory tests. The studies of complex macromolecular systems require the development of proper models and the usage of efficient simulation tools like Dynamic Lattice Liquid model. Due to enormous amount of simulations and extremely long time scales of diffusion modeling they have to be partially carried out on parallel, dedicated computing machines like *Analyzer of Real Complex Systems* (ARUZ) located in BioNanoPark in Lodz.