Molecular Motion, Structure and Surface of Proteins, Membranes and Polymers – Simulation by Dynamic Finite Volume Models (FVM)

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Macromolecular assemblies of domains of different composition occur in proteins, membranes, carbohydrates, nucleis acids and block-polymers. During function, reaction, regulation or work the location and surface exposition of those micro-domains changes, which depicts a molecular motion at the nanometer scale, i.e. a nanoscaled structure dynamics.

The finite volume method (FVM) for simulation and description of macromolecular assemblies by cube models [1,2] was extended to molecular motion. The method and the corresponding PC-program FINIX describes a macromolecular object as an assembly of cubes of equal size, but consisting of up to 255 kinds of matter (domain types). The domain properties, composition, scattering densities, H-D exchange and optical dispersion (X-rays) as well as the surface exposition are stored in tables. The actual location of each micro-domain is given by the resting position and a displacement vector d(t) as function of time. This allows the simulation of molecular motion, i.e. time dependent domain displacements, which result in a variation of surface exposition and distance.

The dynamic finite volume method is used for the simulation and interpretation of time resolved structure investigations of solutions, e.g. Neutron scattering SANS including H-D exchange (contrast variation), X-ray small angle scattering SAXS and anomalous X-ray scattering ASAXS with synchrotron radiation, spectroscopy, labeling and crossliking of flexible macromolecular assemblies, e.g. proteins and membranes. [3,4]

Literatur:

[1] T. Nawroth, *Physica B* **1989**, 156, 493 [2] T. Nawroth, *Habilitation thesis* **1995** University Mainz [3] M. Roessle, E. Manakova, I. Lauer, T. Nawroth, R. Gebhardt, T. Narayanan, H. Heumann, *ESRF Newsletter* **1999** 33, 10 [4]T. Nawroth, M. Rusp , R.P. May, *Physica B* **2003**, submitted