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Multiscale dynamics of biomolecular systems

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The dynamics of biomolecular systems, from small peptides to large multidomain complexes, takes place, both in space and time, at scales that are larger than atomistic but usually smaller than continuum macroscopic. For example, the dynamics of protein conformations constituting protein folding phenomenon is known to include not only the protein's atoms but also a significant part of water molecules surrounding the protein. Temporally this dynamics happens at the nanoseconds to seconds scales. Therefore, understanding how the small scale atomistic motion results in complicated behaviour at larger scales is necessary for uncovering the mechanisms of biomolecular motions. Conceptually, the transformation between the scales for liquid state of matter is only explained for the extremes of the scales: for example, macroscopic properties of the system as a whole are obtained by averaging the atomistic details. The picture is much less clear when the physics at the intermediate scales are considered. Thorough investigation of concepts such as fluctuating hydrodynamics (the fluctuations at the continuum fluid dynamics level are hypothesised to be random processes resulted from the averages over not large enough number of atoms) is only recently started. But this is exactly the time and space scales at which the most important biomolecular motions happen! Are the fluctuations near the protein the same as in pure water? How far from the protein should you take water to have statistically the same fluctuations? Are they random fluctuations at all or something fundamentally different? From this point of view high performance computer simulation is currently reaching the time and space scales at which direct "experimental" verification of these interscale phenomena becomes possible. At the talk I will illustrate such across-the-scales phenomena by examples of small peptides in water.