Modelling and understanding complex biomolecular systems and processes: Applications in nanosciences, biotechnology and biomedicine.

Bogdan Lesyng
Interdisciplinary Centre for Mathermatical and Computational Modelling and Faculty of Physics, Warsaw University
Warsaw, Poland

Protein and nucleic acid folding, enzymatic reactions, functioning of complex biomolecular systems, DNA replication, transcription, protein synthesis, phosphorylation reactions, signaling, cell cycles, are examples of complex biomolecular processes occurring in different space and time-scales. Structures can be predicted using either experimental structure analysis methods, or theoretical approaches "from sequence to structure" prediction strategies. These bioinformatics methods typically include structure-based homology analysis. Mesoscopic approaches are based on the Poisson-Boltzmann and Generalized Born models. In turn, microscopic approaches account for Monte-Carlo procedures, microscopic long-time symplectic classical molecular dynamics, as well as quantum-classical dynamics. Such methods allow, amongst others, algorithmic structure predictions and description of structure formation phenomena, description of specific molecular recognition processes, and analysis of dynamics of complex biomolecular systems and processes, as well as of complex metabolic pathways, including steering and controlling cellular mechanisms.

Such an integrated approach ***(e-science)*** allows ***to understand*** complex biomolecular and cellular structures and processes. This influences positively ***development of practical applications*** such as molecular design, including drug design, and biotechnological and biomedical solutions and strategies.

Integration of bioinformatics, chemical and physical approaches require ***new interdisciplinary educational programs and strategies***. Coupling of higher education and interdisciplinary research is highly required to attack challenging problems in high-quality science and emerging technologies, which favours economical development. It is obvious that computational platforms for carrying out current e-science projects should be based on ***novel WEB and GRID technologies***.

For an overview of multiscale (bio)molecular modelling methods, see e.g. B. Lesyng, *Simulations of Biomolecular Systems and Processes: Perspectives and Limitations,* in: "Modelling and Simulation: A Tool for the Next Millenium", (13th European Simulation Multiconference, June 1-4, 1999, Warsaw), Society for Computer Simulation International, pp. 26-32, (1999).

Acknowledgements: Studies are supported by European Centre of Excellence in Biomolecular Modelling, Bioinformatics and Applications (MAMBA), Warsaw University.