

Monthly informal seminar series on
Integrative Modelling in Biophysics

presented by
Molecular Biophysics Unit, IISc



**Network models in biology:
Molecular machinery, chromosomal dynamics, and missense variants**

Network models have proven to assist in improving our understanding of the coupled dynamics of biomolecules, from individual proteins to supramolecular systems, and even the entire chromatin, in recent years. Among network models that have been developed for biological applications, elastic network models (ENMs) found wide usage in molecular biology. The global motions predicted by ENMs have proven in numerous applications in the last two decades to provide a good description of molecular machinery and allosteric behavior. Application to supramolecular structures, including cryo-EM structures, has been a major utility. More recently, ENMs proved useful to exploring chromosomal dynamics, using data from Hi-C experiments to reconstruct *in silico* the connectivity of the chromatin and provide a physical basis for gene regulation transcription and cell type differentiation. Finally, machine learning algorithms that incorporate ENM predictions provide an improved assessment of the effect of mutations on function, compared to those based on sequence and structure exclusively. These recent developments and future biomedical and pharmacological applications will be discussed.



Prof. Ivet Bahar

Distinguished Professor & JK
Vries Chair Computational &
Systems Biology Dept, School of
Medicine, University of
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Date: 9-Nov-2021 (Tuesday)
Time: 17:30 hours (IST)

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Ivet Bahar is currently a Distinguished Professor and John K Vries Chair at the University of Pittsburgh, School of Medicine, Department of Computational and Systems Biology with more than 300 publications and 27,000 citations in scientific journals, to date. She is known for her pioneering work on the development of elastic network models and multiscale computational methods which helped gain a mechanistic understanding of protein dynamics and allostery. Upon joining the University of Pittsburgh in 2001, she has founded multiple reputed Centers for advancing computational biology (Dept of Computational biology, 2004; Dept of Computational and Systems biology, 2010, etc.). Notably, she co-founded the first Ph.D. degree-granting program in 2005 between Carnegie Mellon University and Pitt, as one of 10 national programs to provide interdisciplinary research training in biomedical, physical, and computational sciences. She served as a reviewer/scientific advisor/executive board member of various national and international scientific organizations like NIH, ERC, and HFSP to name a few. Additionally, she co-founded in 2005 the first PhD degree-granting program between Carnegie Mellon University and Pitt, selected by the HHMI and NIH. Her research primarily focuses on biomolecular systems dynamics; evolution of proteins' sequence, structure, dynamics, and function; network models for protein-protein interactions, supramolecular machinery, and allostery; and computer-aided drug discovery.
<https://www.cccb.pitt.edu/Faculty/bahar/personal.html>