



Biomedical Informatics Grand Rounds

Wednesday, March 20, 2024

3:00 pm – 4:00 pm

System Level Understanding of the Disease with Atomic Details

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Remote Access

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Meeting ID: 956 1719 7636 Passcode: 924293

Bio: Dr. Dima Kozakov is a professor in the department of Applied Mathematics and Statistics at Stony Brook University; he is also an affiliate member of both the Laufer Center for Physical and Quantitative Biology and Institute for Advanced Computational Sciences. He has a MS and BS in Applied Mathematics and Physics from the Moscow Institute of Physics and Technology. He completed his PhD in Biomedical Engineering and was a postdoctoral fellow under Sandor Vajda at Boston University.

Dr. Kozakov research interests lie at the intersection of applied mathematics, physics and computational biology. He focuses on two main goals. The first is the development of mathematically elegant, computationally efficient and physically accurate algorithms for modeling macromolecular structure and function on the genome scale. The second is the application of novel methods to improving the understanding of biological problems and to the design of therapeutic molecules with desired biological and biomedical properties.

Abstract: A proper understanding of disease etiology requires longitudinal systems-scale reconstruction of the multitiered architecture of eukaryotic signaling, including transcriptional and post-translational (PTM) regulation of gene and protein activity in eukaryotic cells, preferably with atomic resolution to identify disease targets as well as rationally design therapeutics to revert the signaling back to normal. In this talk I will describe our efforts on combining mass spectrometry derived multi-omics data with high throughput physics inspired deep learning pipelines to model differential macromolecular interactions in healthy and disease states, focusing on protein-protein and protein-metabolite structural interactions. In the first part of the talk I will talk about our efforts on toolset development for modeling molecular interactions and drug discovery, including new therapeutic modalities such as PROteolysis TARgeting Chimeras (PROTAC). In the second part I will talk about applications of the approach to different disease processes including cancers and Sars-COV2.

Educational Objectives:

1. To learn about integrating mass spectrometry and deep learning models to model macromolecular interactions in healthy and diseased states.
2. Describe a new toolset in modeling molecular interaction, including with new therapeutic molecules like PROTAC.
3. Learn about applications of this approach on different types of diseases like cancer and Sars-COV2.

Disclosure Statement: The faculty and planners have no relevant financial relationship with ineligible companies, whose primary business is producing, marketing, selling, reselling, or distributing health care products used by or on patients.

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