Title:

Great Disruptions and Expectations: A Perspective in Protein Modeling Research

Abstract:

Biology has undergone many revolutions, including Darwin's theory of evolution, the discovery of DNA, the mapping of the human genome, the discovery of the CRISPS-Cas9 genome editing technique, and more. Many disruptions have opened or redirected entire domains of scientific enquiry. Anfinsen showed us that protein tertiary structure was largely encoded in the amino-acid sequence. John Kendrew, reporting on the power of X-ray crystallography, began his feature article in Scientific American in 1961 with now these famous sentences "The way in which the chain of amino acid units in a protein molecule is coiled and folded in space has been worked out for the first time. The protein is myoglobin, the molecule of which contains 2,600 atoms." Seminal work by Scheraga, Karplus, and Levitt motivated decades of computational studies on protein tertiary structure, dynamics, and function. I followed the Nobel laureates' model-based research and designed physics-based models capable of shedding some light into the relationship between structure, dynamics, and (dys)function in small proteins and peptides. Then came the data revolution. Old questions could be reformulated anew and investigated with data-driven and hybrid models. My laboratory showed these models to be more powerful in many respects, yet not always satisfying. And now comes news Alphafold has solved a 50-year grand challenge in biology. Many of us wonder what this means for protein modeling and, for some of us, for our academic and scientific careers. I will argue in this talk that this unexpected yet to be expected disruption is a wonderful opportunity that we can leverage to finally be able to get into the most interesting, complex, and messy questions that molecular biology never fails to provide.

Bio:

Dr. Amarda Shehu is a Professor in the Department of Computer Science in the Volgenau School of Engineering with affiliated appointments in the Department of Bioengineering and School of Systems Biology at George Mason University. She is also Co-Director of the Center for Advancing Human-Machine Partnerships (CAHMP), a Transdisciplinary Center for Advanced Study at George Mason University. Shehu obtained her Ph.D. from Rice University in 2008, where she was an NIH pre-doctoral fellow. Shehu's research focuses on novel algorithms in artificial intelligence and machine learning to bridge between computer and information sciences, engineering, and the life sciences. In particular, her laboratory has made many contributions in bioinformatics and computational biology regarding the relationship between macromolecular sequence, structure, dynamics, and function. Shehu has published over 130 technical papers with postdoctoral, graduate, undergraduate, and high-school students. She is the recipient of an NSF CAREER Award, and her research is regularly supported by various NSF programs, as well as state and private research awards. Shehu is also the recipient of the 2018 Mason University Teaching Excellence Award, the 2014 Mason Emerging Researcher/Scholar/Creator Award, and the 2013 Mason OSCAR Undergraduate Mentor Excellence Award. She currently serves as Program Director at the National Science Foundation in the Information and Intelligent Systems Division of the Computer and Information Science and Engineering Directorate.