Abstrakt:

Recent dramatic advances in modeling of protein structure, attained with the AlphaFold algorithms from DeepMind, and by others, may lead to the conclusion that the long-standing Protein Folding Problem has now been solved. The folding challenge, so elegantly stated by Christian Anfinsen (Nobel Prize in Chemistry, 1972), puzzled researchers in this area for nearly fifty years. But has the folding problem really been solved? Not everyone agrees, for example "The protein-folding problem: Not yet solved", Moore, Hendrickson, Henderson, and Brunger, Science 2022, Feb 4; 375(6580):507. We will examine the recent progress in modeling of protein structure from the point of view of CASP, the Critical Assessment of Structure Prediction experiments. We will also take a closer look at what was accomplished so far, and at the challenges that remain.

Notka:

Krzysztof Fidelis is directly involved in the Critical Assessment of Structure Prediction (CASP) program, dedicated to identifying state-of-the-art in modeling of protein structure. CASP accomplishes this through independent assessment of macromolecular structure modeling methods, with approximately 100 research groups worldwide taking part. He heads the CASP Protein Structure Prediction Center since 1996, instituted to support the organization of CASP, infrastructure, evaluation of predictions, and dissemination of results. Together with other members of the CASP Organizing Committee, he shaped the CASP assessment experiments to address the demands of this rapidly evolving field. He has 30+ years of experience in applied modeling and in modeling methods development, including model assessment and analysis, where he introduced several metrics and formalisms.