SCHOOL OF INFORMATICS AND COMPUTING
CENTER FOR BIOINFORMATICS RESEARCH

# Lukasz Kurgan

## Virginia Commonwealth University

Indiana Memorial Union, Walnut Room
Thursday September 21, 2017, 3:00 PM

### Selection and characterization of targets for structural genomics

**Abstract:** Structural and functional annotation of the rapidly expanding protein universe, defined as a set of all proteins of all organisms, is a significant challenge. Perhaps surprisingly we know very little (less than 1%) about the protein universe. Structural genomics (SG) is a large-scale international effort to solve structures of important biological macro-molecules, primarily focusing on mapping structures of the protein universe. Knowledge of protein structures facilitate understanding of their biochemical and cellular functions and deciphering whether and how they interact with other molecules, including drugs. One of the main bottlenecks in SG is a very low success rate of the production of diffraction quality crystals for the X-ray crystallography, the dominant method for the determination of protein structures. However, the SG pipelines allow for some flexibility in the selection of protein targets. This motivates development of computational methods for the prediction and assessment of the crystallization propensity of proteins, with the underlying goal of finding easier to crystallize and functionally equivalent protein targets. We will overview the currently available computational predictors of crystallization propensity. We will focus on one of our newest methods, fDETECT, which provides relatively strong predictive performance coupled with short runtime. Utilizing fDETECT and other tools, we will answer the questions of how many protein structures across the protein universe can be determined with the help of the X-ray crystallography and computational modelling, and whether the putative propensity for crystallization can be also used to predict resolution of protein structures.

**Biography:** Lukasz Kurgan received Ph.D. in computer science from the University of Colorado at Boulder in 2003. He joined department of Computer Science at the Virginia Commonwealth University in 2015 as the Qimonda Endowed Professor. Before that he was a Professor of Electrical and Computer Engineering at the University of Alberta. His research interest are in (un)structural bioinformatics of biologically interesting macromolecules, from individual proteins and small RNAs to complete proteomes and transcriptomes. Dr. Kurgan is an Area Editor for structural bioinformatics of *BMC Bioinformatics* and Associate Editor of several journals including *Intrinsically Disordered Proteins*, *Neurocomputing*, and *Current Protein and Peptide Science*. More details are on the web site of his lab a http://biomine.ece.ualberta.ca/

SCHOOL OF INFORMATICS AND COMPUTING
INDIANA UNIVERSITY
Bloomington