

Data Science for Drug Discovery

Engineered proteins are synthetic novel proteins (not found in nature) that are designed to interact with a specific biological function. Such proteins can be used for the design of novel drugs such as new Biologics. We present a massively parallel Data Science computational tool for the in-silico design of synthetic proteins that interact with a given target protein in order to inhibit the target's cellular functions while leaving non-target proteins unaffected (to minimize side-effects).

Our computer-generated novel proteins have been synthesized in the lab and their inhibitory properties have been verified through experimentation. Applications include: (1) novel synthetic peptides that detect and inhibit the SARS-CoV-2 spike protein, (2) novel synthetic anti-Zika virus peptides, (3) novel synthetic peptides to support stem cell therapy for Muscular Dystrophy, and (4) the identification of a candidate gene for a novel maturity locus in soybean (in support of an Agriculture Canada project to create new soybean varieties for cold climates).

About the Facilitator

Professor Dehne received a MCS from RWTH Aachen University, Germany and a PhD in Computer Science from the University of Wuerzburg, Germany. He is currently a Chancellor's Professor of Computer Science at Carleton University in Ottawa, Canada.

Professor Dehne specializes in interdisciplinary and collaborative research in data science and parallel computing. He employs cloud computing systems, cluster computing, multi-core processors, and GPUs to create new high-performance computing systems for solving data-intensive and computationally hard problems in bioinformatics, business data analytics, and computational engineering. Professor Dehne has published 180+ research papers with more than 6,000 citations.

From 2015 to 2022, he was the Founding Director of Carleton's new Institute for Data Science. Professor Dehne served on the Editorial Boards of IEEE Transaction on Computers, Information Processing Letters, Journal of Bioinformatics Research and Applications, and Int. Journal of Data Warehousing and Mining. He is a member and former vice-chair of the IEEE Technical Committee on Parallel Processing, and a member of the ACM Symposium on Parallel Algorithms & Architectures Steering Committee. From 2010 to 2020, Professor Dehne was a Fellow of the IBM Centre For Advanced Studies in Toronto, Canada.

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