Centre for Research in Molecular Modeling (CERMM) Seminar Series

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Molecular Simulations of Intrinsically Disordered Proteins

Intrinsically disordered proteins (IDPs) are abundant in all kingdoms of life and fulfill many critical functions. Despite their biological importance, IDPs are poorly understood relative to the wealth of structural information available for folded proteins. The structural description of IDPs poses formidable challenges to both theory and experiment: IDPs do not have a stable structure, but rather a structural ensemble consisting of many interconverting conformational states. Molecular simulations can be used to obtain structural ensembles of IDPs, but are currently limited by the accuracy of their energy functions (force fields). To address this challenge, we have carried out a systematic comparison of state-of-the-art force fields for the specific case of IDPs, and developed an improved force field suitable for both IDPs and folded proteins. Accurate simulations of IDPs open up new possibilities for the detailed structural characterization of this important class of proteins. As a prototypic example of the insight afforded by molecular simulations of IDPs, I will describe our work on the structure of elastin, the protein responsible for the elasticity of skin, lungs, and arteries.

Sarah Rauscher completed her undergraduate degree with honours in Astrophysics with a minor in Chemistry at McMaster University. She did her PhD at the University of Toronto. She did Postdoctoral Fellowships at the Hospital for Sick Children and at the Max Planck Institute for Biophysical Chemistry in Göttingen. Since 2017, she is Assistant Professor in Physics at the University of Toronto.