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Voronoi Tessellations Shell Analysis SARA CHENG, University of Texas at Austin, CAMPBELL COMPTON, HOA NGUYEN, KELVIN CHENG, Trinity University, TRINITY UNIVERSITY PHYSICS AND TRINITY UNIVERSITY MATH COLLABORATION — In studies of lipid bilayer systems, disruptions caused by interaction of protein with lipid components are difficult to quantify. The purpose of our research project is to develop an analysis suite to analyze molecular dynamics (MD) trajectories of beta-amyloid on lipid bilayer systems containing POPC and cholesterol lipids. Using a combination of Python, Shell, and MATLAB scripts, we analyze multi-component, multi-shell, and multi-frame systems in order to better understand how beta-amyloid affects neuronal membrane mimics. The overall goal of our project is to gain insight on the damage caused by beta-amyloid and its role in the parthenogenesis of Alzheimer's disease. The focus of our presentation will be on the post-processing shell data generated from running our MD simulation results through a computer program, Voro++, which involves using Voronoi Tessellations generate shells around the protein. We will describe our method of extracting and analyzing MD simulations, including post-processing the results generated by a combination of GROMACS tools and in-house scripts. The results of our analysis suite, with a focus on density and order parameter, indicate strongest disruption of the lipid bilayer in the first shell surrounding the protein.

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