1154-92-2511 **David F. Snyder*** (ds08@txstate.edu), MCS 470, Department of Mathematics, Texas State University, 601 University Drive, San Marcos, TX 78666. *On the Dynamics of Solvent-excluded Surface Topology under Protein Flexing.* Preliminary report.

The solvent-excluded surface (SES) of a protein has a significant role in a protein's solvation, folding, and function. Accurate quantitative relationships between these features remain mostly unknown. The Protein Data Bank (PDB) protein database contains over 100,000 sets of coordinates, but only slightly over 10,000 unique protein chains. The PDBFlex database (http://pdbflex.org) provides free public information on the flexibility of protein structures as revealed by the analysis of variations between depositions of different structural models of the same protein in the PDB. Using protein clusters as identified in PDBFlex, we compute the persistent homology of the solvent-accessible surface of each conformation within a given protein cluster, to investigate the dynamics of the surface topology as the structure flexes through its different conformations. Mathematically, we are computing the Leray sheaf $\mathcal{H}^*[\pi]$ of a map π which is (generically) a surface bundle over a space of rigid embeddings of a simplicial 1-complex in euclidean 3-space. We demonstrate the results for a couple of protein clusters of biomedical interest and discuss potential applications. (Received September 17, 2019)