**Abstract**

With modern technology and High Performance Computing (HPC), Molecular Dynamics (MD) simulations can be both task and data parallel. That means, they can be decomposed into multiple independent tasks (i.e., trajectories) with their own data, which can be processed in parallel. Analysis of MD simulations includes finding specific molecular events which induce conformational changes. Every state comprises of k + 1 paired trajectories. Our method is robust regardless of the type of protein, sampling rate, number of trajectories from different proteins and mutants listed below.

**Our Method**

We use domain knowledge to determine the residues of interest 'r' (i.e., residues Structural Rearrangements, Binding Events, Protein Associations are some conformational changes). With this knowledge, we identify different states of the protein through its trajectory. Additionally, we are able to explain which residue-pair contributed the most for a molecular event. Our algorithm can monitor molecular events in a protein trajectory in -Situ. With this knowledge, we identify different states of the protein through its trajectory. Additionally, we are able to explain which residue-pair contributed the most for a molecular event. Our algorithm can monitor molecular events in a protein trajectory in -Situ.

**Evaluation and Results**

We validated our results with respect to TICA and with the expected conformation changes determined by domain scientists. Figures 6-8 demonstrates our results for trajectories from Globulin and Figs 9-12 for E50K.

**Conclusions**

Our method shows a behavior that is consistent with TICA. But unlike TICA, the analysis can be performed in the same node as the simulations or run concurrently on different nodes, saving time and computational resources. We train an ensemble of lightweight ML models that do not require the entire view of the protein to determine the relevant changes.