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Research Area: Computational Science and Mathematics

The project aims to use Visual Molecular Dynamics for displaying, animating, and analyzing large molecular systems using 3-D graphics and built-in scripting. Using various software and experimental data, calculations are made to analyze the trajectory of a molecular dynamics (MD) simulation; enabling interactive display and animation of such molecular structures as proteins, nucleic acids, and lipid assemblies. The project thus, uses Molecular Dynamics software to load large, complex molecular systems into the simulation programs and get a 3D representation of the simulated system, which can then be manipulated to get a variety of views.

Specific subtasks:

1. To perform a molecular and stochastic dynamics computation on specific molecules
2. Run programs with the desired temperature, pressure and solvent to analyze chemical effects
3. Use specific thermodynamic ensembles with trajectories that are propagated using a velocity integration method
4. Implement desired number of dynamic steps and time intervals for different environmental conditions

Research mentor:

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