A tool for exploratory data analysis of time series data from molecular dynamics simulations

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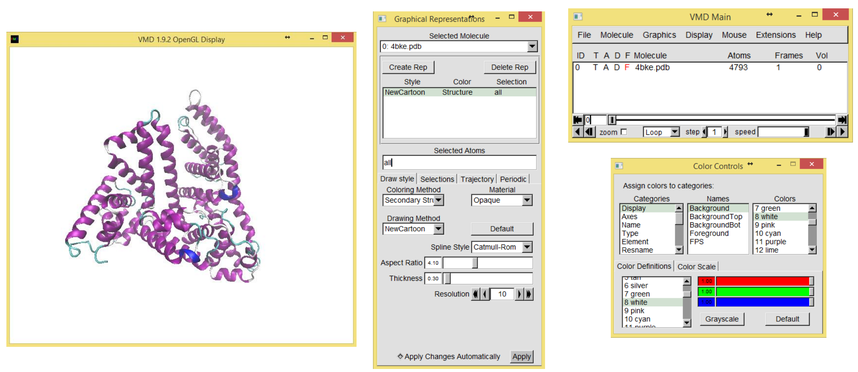
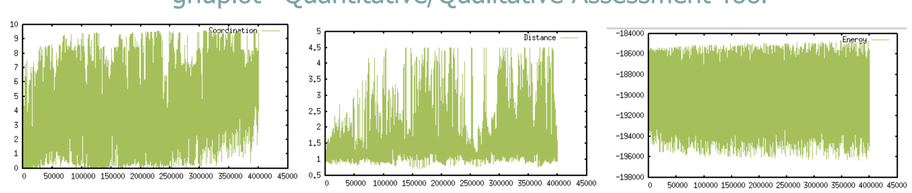
Problem and Motivation

Problem - Current visualization tools for molecular dynamics simulations focus on representing structural aspects - like secondary structure of protein, charge, atom type - at every timestep of the simulation. Relating crucial information – like energy, pressure – to the structure is necessary for a holistic assessment of the simulation trajectory.

Visual Molecular Dynamics – Qualitative Assessment Tool



gnuplot– Quantitative/Qualitative Assessment Tool



Approach

Build an exploratory data visualization platform that promotes comparison of quantitative and structural data generated from molecular simulations and reduces switching time between software for the same.

Processing Algorithms

Distance Matrix	Values are scaled between [0,1]. Euclidean distance between points are calculated.
Multi-dimensional scaling (MDS)	Points are projected on a 2-dimensional plane by a classical MDS algorithm which operates on the distance matrix.
Removing overlap	Overlapping points are moved away using a random number generator

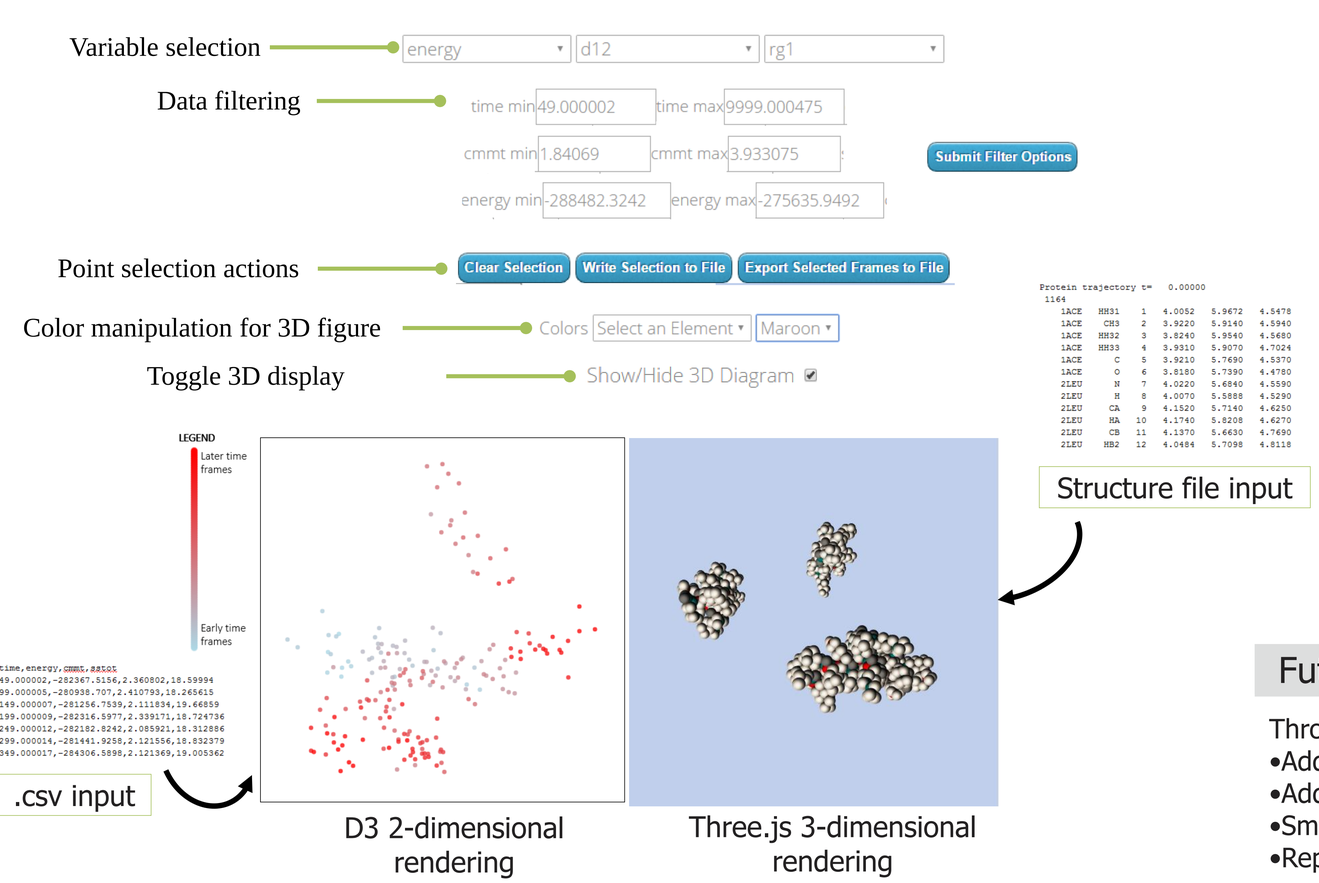
Interaction

Zooming	Cartesian fisheye zooming with distortion is implemented
Point selection	An invisible point-in polygon selects points as the user drags the mouse
Filtering	User defined ranges for all variables can be selected

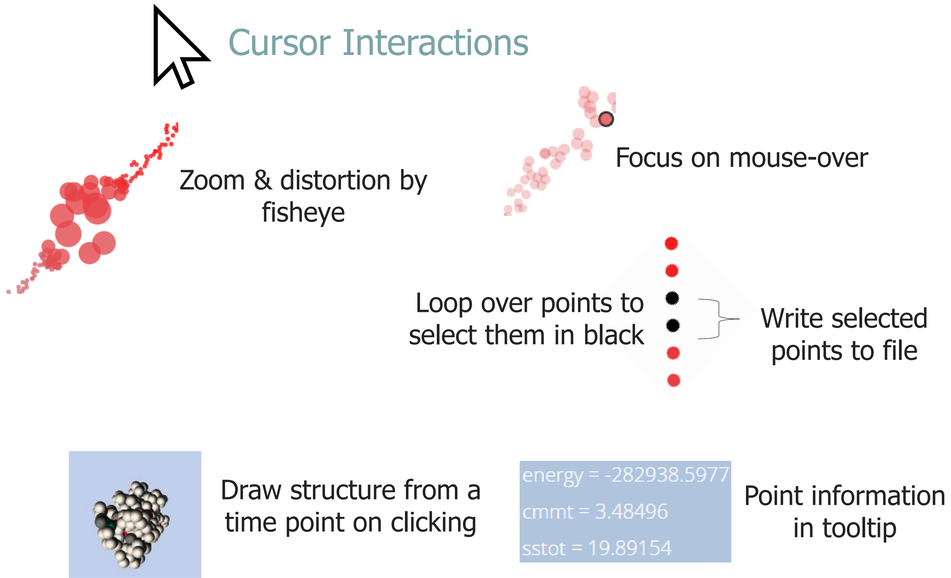
3D Structure Mapping

Spheres-only Model	Atoms are represented by colored spheres. Bonds are not represented
Animation	Rotation and zoom are implemented on the 3D structure
Perspective Camera	Perspective, rather than Orthographic camera, is used to include depth perception

Results



Cursor Interactions



Future Work

Through user studies it is evident that there can be a number of extensions of this project:

- Adding more 3D representations, clustering algorithms
- Adding options to export image for collaboration
- Small multiples view of structure, and graphs
- Repurposing this to project points on a contour plot or "energy surface"