Protein Flexibility Analysis: a Friendly Interface
Yang Li, Smith College, Northampton, MA
Faculty Adviser: Ileana Streinu, Computer Science Department, Smith College

Introduction

Motivation
- Proteins are flexible structures that exhibit internal motions.
- Protein flexibility analysis helps scientists understand protein function and facilitates new therapeutics for diseases.

About RigDyn
- A research software package for flexibility analysis of general structures, such as proteins.
- Uses rigidity theory to provide information on rigid regions of proteins.

Project Goal

Problems
- The first version of RigDyn was difficult to use for non-computer scientists.
  - It was command-line driven and had to be invoked by manual editing of configuration file
  - Analysis output was not easily comprehensible for human viewers.

Solution
- Design a user-friendly interface that integrates input configurations and analysis outputs.
- Maximize the usability of RigDyn for users at all levels

Interface Overview
- A web-based GUI (Graphical User Interface) primarily designed for protein flexibility analysis.
  - Runs on a server, thus avoids the hassle of installation.
  - Focuses on three aspects: the front-end, the viewer and the user interaction.

The Front-end

The front-end allows users to invoke RigDyn with a few clicks. Different inputting and running options are organized into expandable sections.

User Interaction

- Flexibility analysis can be easily re-run with adjusted configurations.
- Users may add constraints between a pair of atoms, and observe how rigidity structures change from previous results.

The Viewer

Numerical analysis outputs are transformed into graphical representations via Jmol, a 3D biomolecule viewer. The viewer is accompanied by interactive controls that can manipulate the visualization based on user’s needs.

Future Work

- Continue to enhance user-friendliness
- Test and verify the viewer with a larger data set.
- Stabilize its compatibility with different web browsers to prepare for actual release.

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