Contact Map Trajectory Viewing Tool

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Abstract

`ProtCon` is a java-based computational tool for display and analysis of macromolecular residue-residue contacts and their time-evolution during an MD simulation. It takes time-ordered sequence of PDB files on input and produces a dynamical set of contact maps.

Keywords: Contact Map, Molecular Dynamics Trajectory, Folding

1 What is ProtCon ?

The Contact Map Viewer gives researchers with the ability to visualize the evolution of residue-residue contacts in a macromolecule in the course of molecular dynamics simulation. The viewer allows both distinct trajectory overlays and independent control of contact sequence animation. The Contact Map Viewer differs from many other contact mapping tools because it allows multiple contact maps to be viewed simultaneously in the same context.

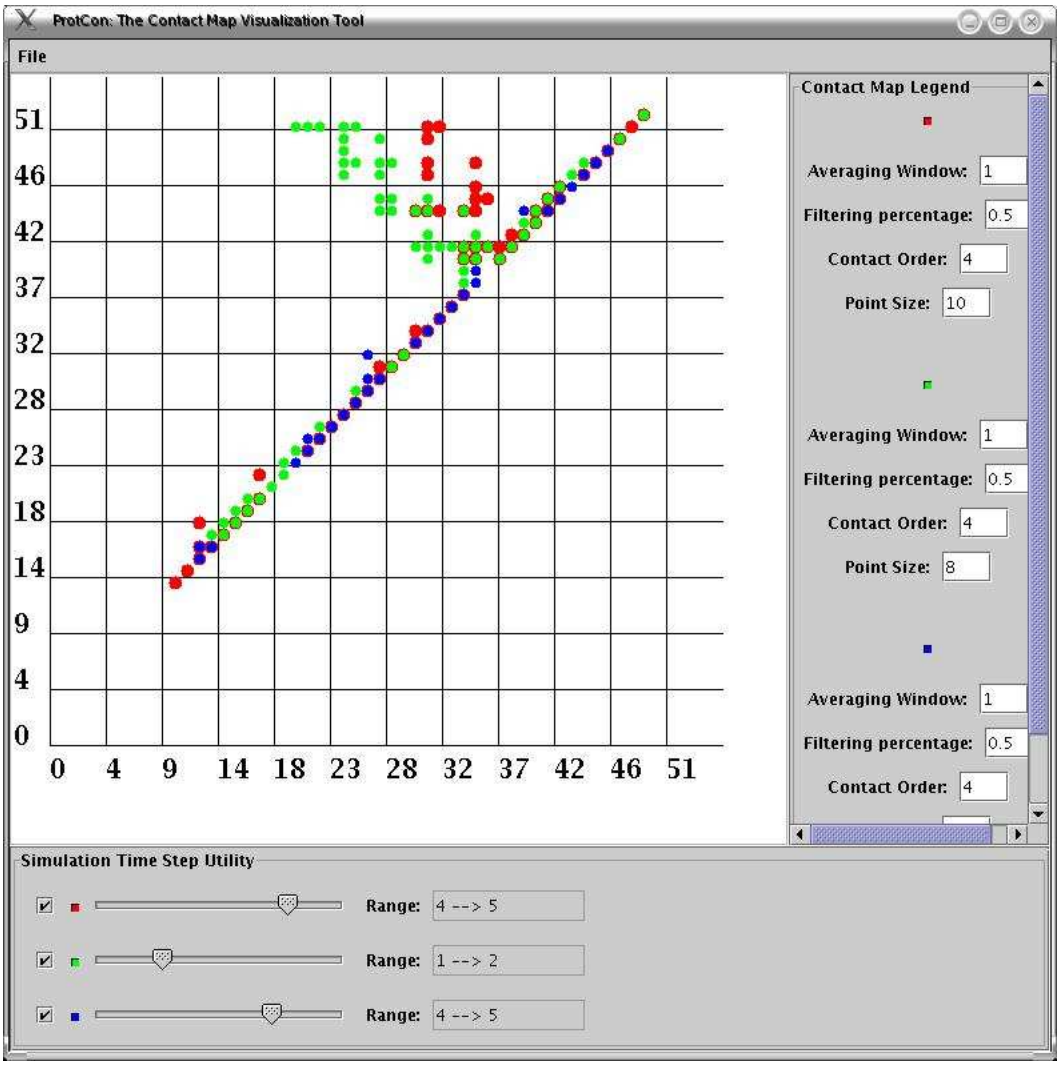

Figure 1: ProtCon : Dynamic Residue-Residue Contacts Visualization Utility

2 Uploading a Trajectory

The process for adding a trajectory is now fully incorporated into the GUI. To add a new trajectory to the contact map, select the menu option $File \rightarrow Open$. A file selection window will appear. The file selection window allows many files to be selected at the same time. Use `Ctrl` or Shift to select all of the PDB files that you would like to be included in a single trajectory. Please use PDB files with only one model for each file.

3 Saving a Contact Map Image

Use the $File \rightarrow Save$ option in the menu to open s save file selection window. Select the location where the file is to be saved by navigating in the window. Add a file name in the lower text field. Finally, press save to save your contact map in *.eps* (Extended Post Script) format.

4 Contact Definition

A contact map is a graph indicating the residues in contact in a protein. To qualify as a contact, the minimum atom-atom distance between two residues must satisfy a (user-controlled) criterion. Here, the following one is used: $min\{r_{ij}\} < R_i + R_j + 2R_w$, where r_{ij} is the distance between atoms i and j, R_i, R_j are their respective radii, and R_w is the probe (water) radius. By default, `ProtCon` uses *Bondi* radii set specified in the `atomRadii` file. However, the user can re-set these values in the `atomRadii` file, amounts to specifying a different definition of residue-residue contact. For example, setting $R_w = 0$ will lead to a very stringent criterion for the contacts. The color of the points corresponds to the color assigned to the trajectory. Grid numbering and spacing is automatically calculated.

When new trajectories are loaded, the size of the contact map will automatically adjust to accommodate the largest protein residue count or the largest sequence amino acid count.

4.1 Contact Map Legend

The contact map legend serves as a property list for each trajectory. The trajectories name and color is indicated on the same line.

Next, a text field allows the user to select the window size. The window size indicates the number of frames to be included in a contact map. A greater window size allows the user to identify persistent contacts in the protein. To be a non-volatile contact, the contact should appear in many frames in the window under consideration. By default, the window size is only a single frame.

The filtering probability will dictate in how many snapshot a contact must occur to be put on the map. By default, the value is 0.50. The value 0.50 indicates that a contact must appear in greater than half of the snapshots to be shown. The range for this value is 0 to 1.

The contact order text field allows the user to remove short range (*e.g.* diagonal) contacts from the contact graph. A greater contact distance allows users to focus on long range contacts in the protein. Indicating that residues in contact with adjacent residue s are included in the contact map, the default contact order distance is 1, that is all contacts are shown.

To set trajectories apart from each other and to facilitate trajectory overlays, the point size controls the size of points for a entire trajectory. This feature will allow you to compare trajectories to each other simultaneously.

4.2 Controlling the Time Step

The simulation time step utility allows users to step through their trajectory in an animated fashion. For each trajectory, a slide bar gives the user dynamic control over the contact map in view. Allowing the user to adjust contact map for each trajectory independently, the slide bars for each trajectory are different. To the left of the trajectory title, a check box allows the user to hide a particular trajectory from view. Additionally, the label to the right of the slider indicates the trajectory frames currently visible.

5 Usage Scenario

A researcher generated two protein folding trajectories, under different conditions. One trajectory has lead to a compact native state, while the other one has not. A step-by-step comparison of the time-evolution of the contacts formed during folding may help understand why.

5.1 Necessary Packages

Java JRE 1.4

5.2 Command Format

```
java -jar ProtCon.jar
output:  A 2D graphical representation of residue-residue contacts
compatibility:  All platforms
```

5.3 Input Data

`ProtCon` takes a series of PDB files on input. The PDB files should contain only a single model, with residues numbered sequentially. As naming conventions are diverse, we cannot rely upon file naming for time step ordering. However, we attempt to construct an ordering of pdb files by looking for the first number in the file name. Please note that this ordering may not be lexographic.