

A Distributed Protein Visualization Application

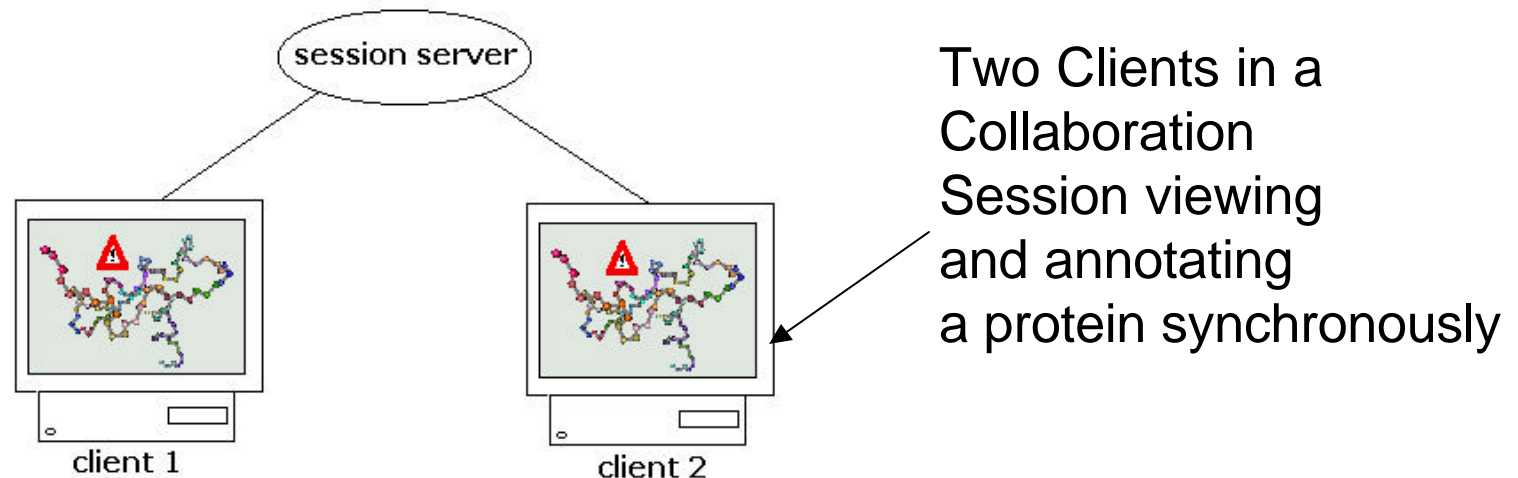


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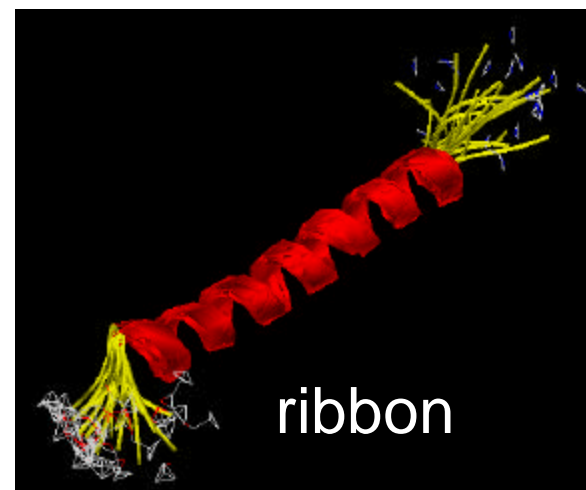
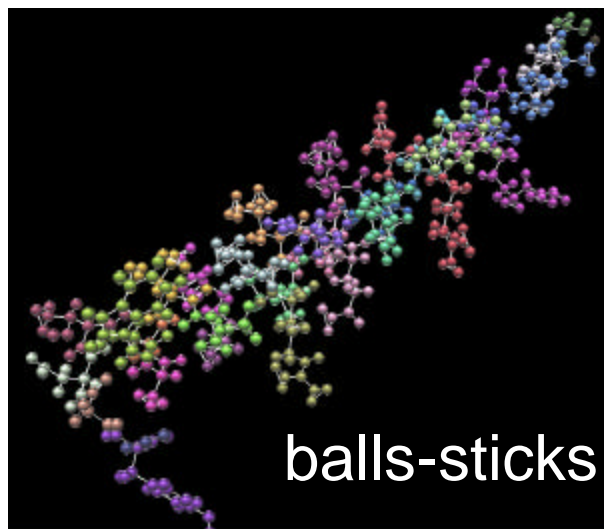
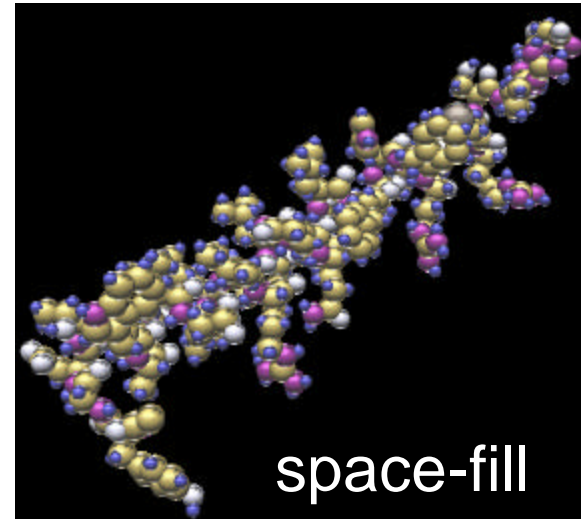
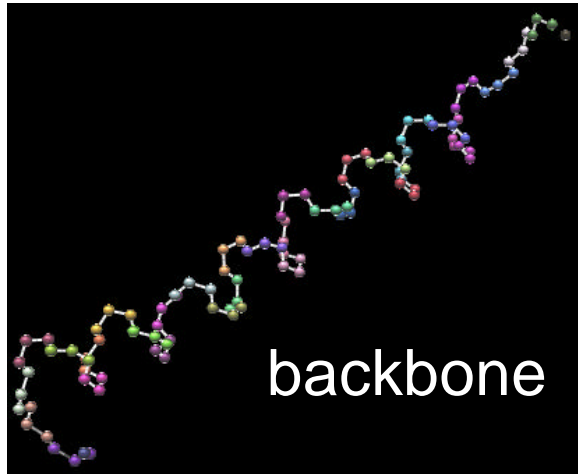
OVERVIEW

- A distributed protein visualization environment supporting collaboration by:
 - Sharing Views
 - Annotation Mechanisms
 - Sticky Notes



VISUALIZATION

- Currently supporting four 3D model types



INFORMATION WINDOWS

Molecule Info

MOLECULE NAME: SERINE PROTEASE INHIBITOR

NUMBER OF RESIDUES: 40

AA Sequence: DAEFRHDSGYEVHHQKLVFFAEDVGSNKGAIIGLMVGGVV

Secondary Structure: TTTTTHHHHHHHHHHTTTTTHHHHTTTT

SELECTED ATOM: NE (Chain No: 1 Group No: 5)

Sequence View
-dynamically updated
during interaction

Tree View
-provides a
hierarchical
interaction

Tree View Mode : Secondary Structure

Change Mode

Molecule : SERINE PROTEASE INHIBITOR

- TURN
- HELIX
- TURN
- HELIX
- ILE
- N
- CA
- C
- O
- CB
- CG1



COLLABORATION

■ Sharing the views

- The 3D view of the molecule is synchronized among users.
- Two modes exist:
 - Master-Slave: only one user is allowed to change the view. Useful for education purposes
 - Peer-peer: Any user can change the view. A Basic Locking Mechanism is implemented

■ Sticky Notes

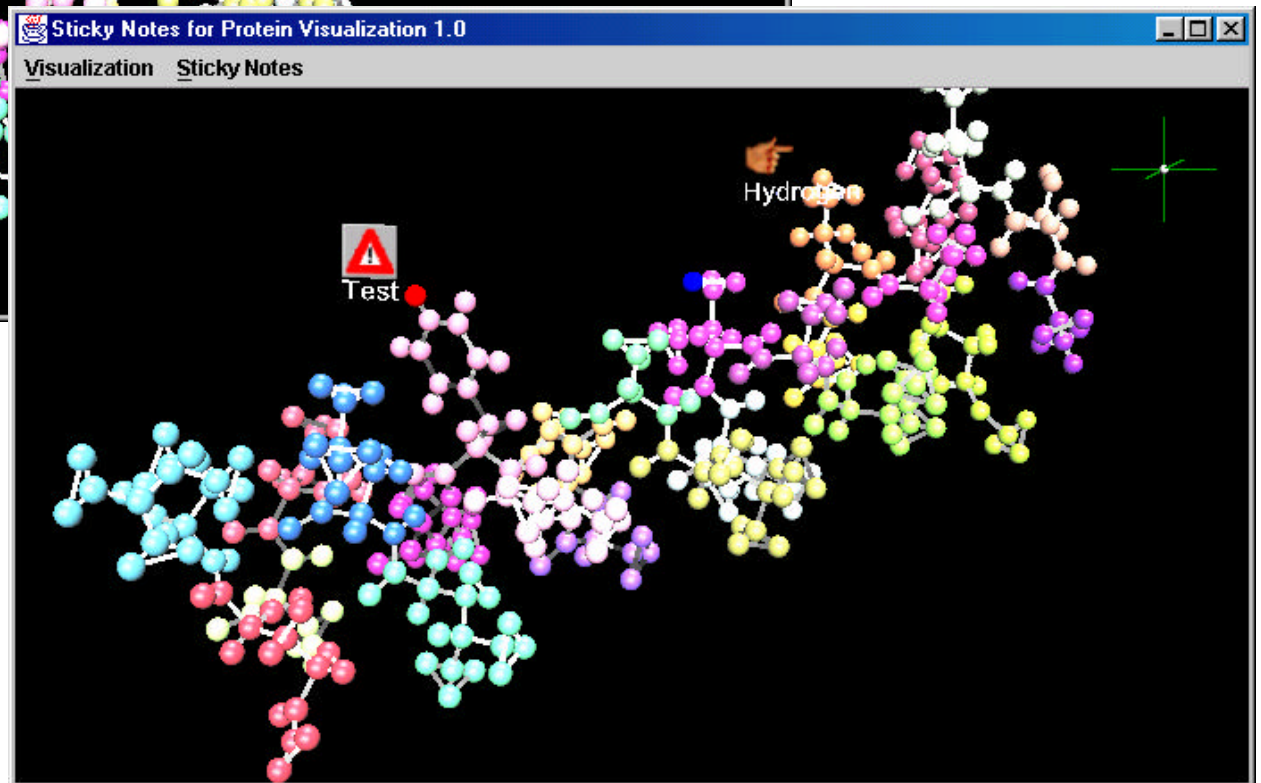
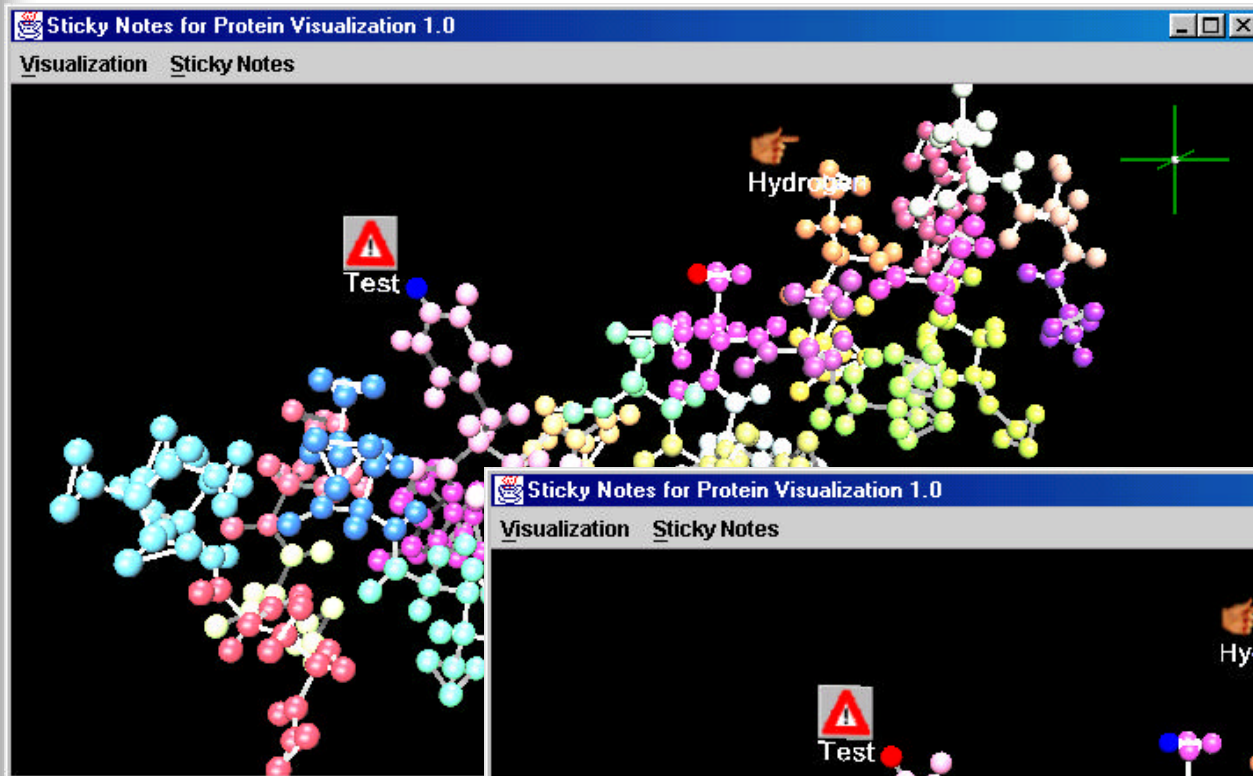
- They provide a mechanism for annotating parts of interest



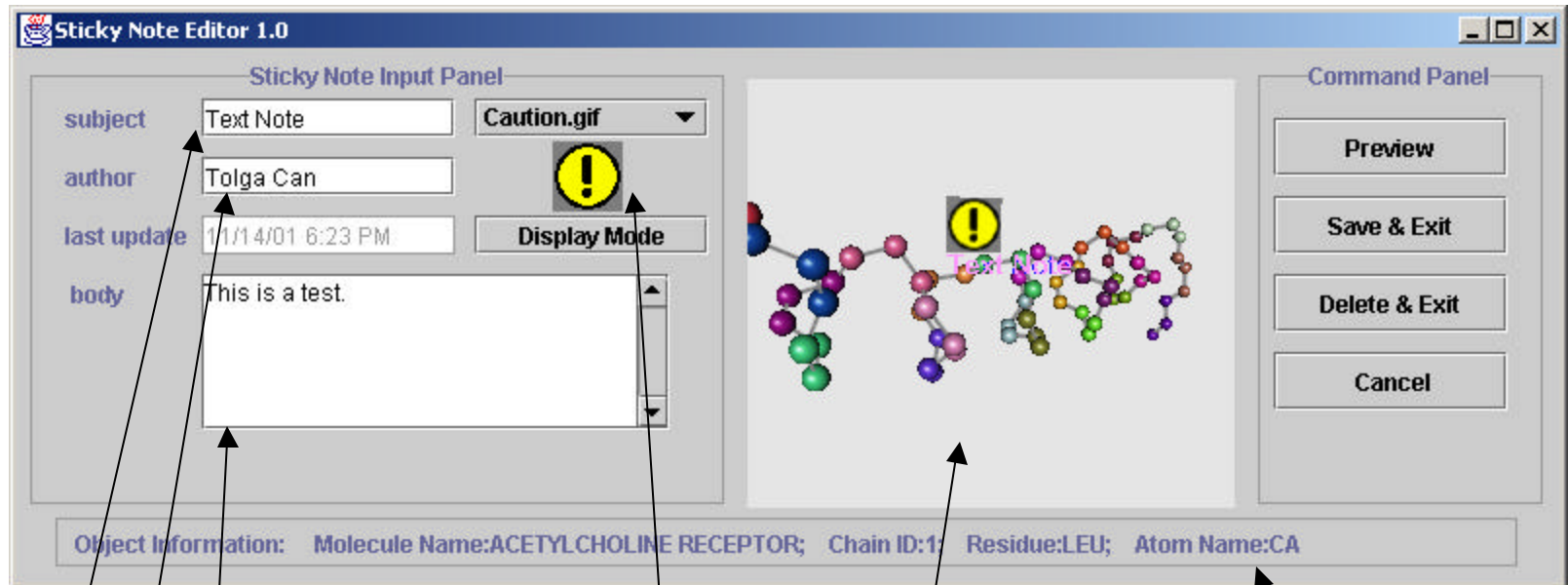
STICKY NOTES

- Annotations that attach to the underlying 3D model
- Different types of notes
 - Basic Notes (Contain Information)
 - Text Notes
 - Audio Notes
 - Advanced Notes (Perform Actions)
 - Action Notes
 - Active Notes
- Situation Awareness (Adapt to environment)
 - Adapt size so that they are always seen easily by the user
 - Adapt orientation so that they are always oriented towards the user
 - Selection of fields for display (title, author, icon, etc.)

A SNAPSHOT OF A SESSION



STICKY NOTES INTERFACE



Selection of Icon

The editable fields of the note:

- subject
- author
- body

Preview Panel

Information about the associated object is stored with the note

ACTION NOTES

- Notes capable of performing actions
 - Change view point, execute an external program, etc.



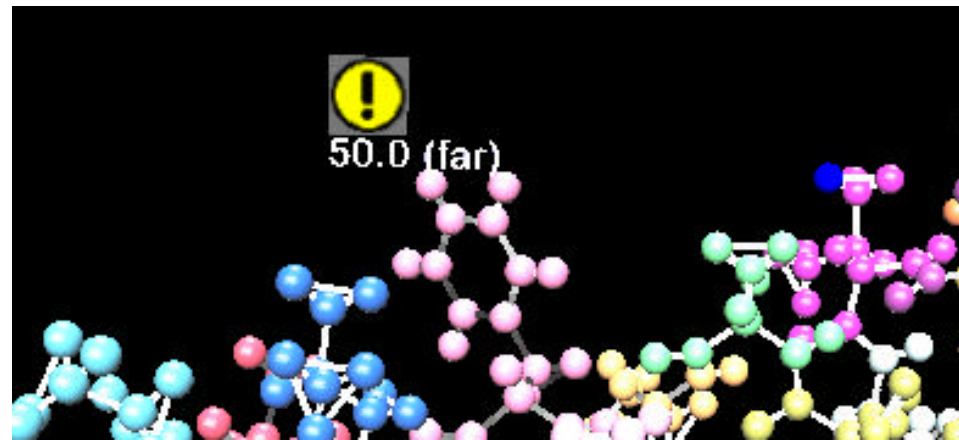
Search PDB information in PDB site



Search for another molecule and display it

ACTIVE NOTES

- Notes that monitor the environment for triggering conditions,
e.g. a note calculating the distance between the model and the view point



- Difference between action notes:
 - They are not user initiated, they are activated by certain environmental changes.



FUTURE WORK

- Add new 3D model types
 - Electron density map
 - Solid surface representation
- Collaborative Protein Modeling
 - Incorporating a protein folding algorithm to enable modeling a protein molecule from scratch or modifying existing proteins
- Notes Management
 - A better note browsing mechanism
 - Supporting user access rights