Concurrent interactive visualization and handling of molecular structures over the Internet in web browsers

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Abstract. This preprint presents a web app (essentially a web page-based program) with which two or more users ("peers") can view and handle 3D molecular structures in a concurrent, interactive way through their web browsers. This means they can share orientation and zoom, commands and other operations in almost real time over the Internet, with the comfort of standard web pages. This web app, open source and built with the open source components JSmol and Peer.js, provides by itself a practical tool for online collaboration and teaching at a distance. More broadly, it illustrates the strong integrability of libraries and technologies for client-side web programming, and opens the way for similar web apps for concurrent work in other disciplines. The web app is available at: http://lucianoabriata.altervista.org/jsinscience/concurrent-jsmol/concurrent-jsmol-visualization.html

Keywords: JSmol, Peer.js, web socket, molecular modeling, structural bioinformatics, web technologies

Concurrent visualization and handling of molecular structures over the Internet is potentially useful for collaborations and teaching at distant locations. A possible way to achieve this is through screen-sharing programs; however, this has a number of disadvantages. First, large amounts of video have to be streamed over the Internet, resulting in decreased quality of the molecular graphics for the receiving peer. Second, there is a possibility that confidential information be captured as the video streams through Internet. Third, and probably most important, the receiver has no control over the visualization. All these shortcomings are addressed by the prototypical web app (program embedded in a web page1,2) introduced here, which uses simple methods and existing web software to provide a unique experience for concurrent molecular visualization and handling over the Internet. As provided, the web app is based on the JSmol3 and Peer.js4 libraries for molecular visualization and connectivity, respectively, but other libraries could be used too. (For the user this is anyway irrelevant because no software needs to be installed and the web app works in any standard web browser.)

Brief Description for Users

Essentially, this web app provides direct browser-to-browser connectivity to transmit states and commands between users. This way, a user can for example rotate or zoom the structure on screen and induce the same rotations and zooms on the screens of other users. Likewise, a user can run a JSmol command on his/her visualization and apply the same command on all the other users’ visualizations. Since the system transfers only small pieces of text-like information about states and commands, but no graphics, the experience is very fluid even over average Internet connections. Also, the molecular files loaded by each user are never sent over Internet, protecting privacy.

Figure 1. Scheme depicting how this web app allows a user to work on a molecular representation and send states and commands seamlessly to the other users, yielding a smooth, computationally inexpensive collaborative experience where the receiver user can also effectively intervene.
To use the web app, each user (or “peer”) must direct his or her browser to http://lucianoabriata.altervista.org/jsinscience/concurrent-jmol/concurrent-jmol-visualization.html. When each user’s page loads, he or she gets assigned a random “PeerJS ID”. At least one user ID must be communicated to the other users (by e-mail or any other medium). When the other users receive the ID of this “master user”, they use it to connect to him/her. This establishes a first connection between the master user and the other users. Since then, users can select whether they transmit rotations, states and JSmol commands to the master user as they apply them to their visualizations, and whether they apply to their visualizations the rotations, states and commands received from the master user. Next, if needed, any other pairs of users can additionally connect to each other to send and receive states and commands directly between them.

Within the web app, users can also chat and send files to each other. And although not implemented in this web app, the communication technology employed also allows the incorporation of video and audio conferencing.

**Brief technicalities about the implementation**

This web app is self-contained in a single HTML file. It uses web sockets (here through the Peer.js library, but others could be used) and a plugin-less molecular viewer for browsers (here JSmol, but also other scriptable viewers could be used). Through HTML and JavaScript code, the web app controls when it sends rotations and commands applied on one peer’s browser to the other peers, and whether the rotations and commands received from another user are applied.

The current implementation runs only over http, but web socket libraries that handle https could be used to allow https access (which would enable JSmol to directly load structures directly from the Protein Data Bank, instead of the user having to download it first).

A last important point is that the web app, as provided in its single HTML file can be directly copied to any other webserver, and should be functional (a copy of JSmol and proper reference to it must be given).

**Perspectives**

Being this web app just a prototype to show feasibility, there are multiple modifications and additions worth exploring. For example, it could be useful to transmit not only commands typed for the JSmol applet but also any other command applied directly from the JSmol interface or console. Also, additional commands prebuilt into buttons could be implemented, depending on the intended uses (small molecules or biological molecules or materials, for research or didactic, etc.)

It is also important to highlight that this example application shall promote the development of interfaces for concurrent work in other disciplines. Not only for molecular sciences but for virtually any discipline where transmitting small pieces of data to transform views on other users’ devices can help to better communicate ideas and concepts at a distance.

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