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Articles

Biomolecules in the Computer

Jmol TO THE RESCUE

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Jmol is free, open source software for interactive molecular visualization. Since it is written in the Java™ programming language, it is compatible with all major operating systems and, in the applet form, with most modern web browsers. This article summarizes Jmol development and features that make it a valid and promising replacement for Rasmol and Chime in the development of educational materials, as well as in basic investigation of biomolecular structure. The description is set up by comparison with the well known abilities of Rasmol and Chime. Jmol is suitable for molecular model display and analysis in biochemistry, molecular biology, organic and inorganic chemistry, crystallography, and materials science.

Keywords: Molecular models, Jmol, Chime, open source, proteins.

BACKGROUND

The use of molecular models on a personal computer is nowadays commonplace, thanks to the availability of easy-to-use software (two inspired historical reviews have been written by Voet [1] and Martz and Francoeur [2]). This pedagogical tool offers several advantages, as compared with classical physical molecular models, among which we can highlight:

- It allows molecular models to be displayed in front of a wide audience, by means of multimedia projectors in the classroom or lecture hall. Also, students are more likely to have individual access to a computer than to a physical model for each molecule.
- It offers unlimited availability of "items" (atoms, bonds), helping one to avoid running out of materials, which frequently occurs with plastic models.
- It is inexpensive.
- It allows the use of diverse representations of a molecule: wireframe, sticks, balls and sticks, spheres (space-filling) and, crucial for proteins and nucleic acids, schematic renderings (such as several variants of ribbons and cylinders and the structures usually dubbed "cartoons").
- Of course, it offers three-dimensional perception, through the possibility of rotating the model in any direction, both automatically and through manipulation by the user. To this end, some programs add lighting, shading, and perspective for a depth effect.
- Most notably, the models are interactive, in the sense that the user (and the instructor programming the materials) can choose all sorts of actions to be performed on the model: the aforementioned rotation, changing the rendering, focusing on a part of the molecule, measuring its geometry, and so forth . . .

REFERENCE SOFTWARE

Many programs exist that allow one to view and manipulate molecular models, both commercial and free. This article does not pretend to review all of them, but instead will focus on two that are available for free and have been extensively used during the last 10–15 years, becoming fairly de facto standards, and a recent one that promises to become an advantageous replacement for them.

First of all is *Rasmol* (by Roger Sayle [3, 4] and later by Herbert Bernstein in the form of *OpenRasmol* [5, 6]), a standalone program running under Unix/Linux, Windows, and MacOS operating systems. It is fast in operation, remarkably low on system requirements (the executable file is only 342–473 kb, depending on the version), and endowed with an extensive command language ("Rasmol scripts") that allows interaction with the molecular model (for a review, see Refs. [6] and [7]). Its extensive spread among the scientific and teaching communities is well known and needs no further explanation here.

Chime was an implementation of Rasmol code in the form of a web browser plug-in, done at MDL (Molecular Design Limited, currently Elsevier MDL [8]). This allowed one to put molecular models inside web pages [9] (initially for viewing with Netscape 3 and 4, later with Microsoft Internet Explorer, too). Although proprietary and copyrighted, Chime has been available for free after registration with MDL.

The ability to create a model in a predefined rendering, surrounded by descriptive text and material, including controls interacting with the model, all of it available through an intranet or the internet, has led to the creation

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through the years of innumerable tutorials and educational websites using Chime (see Ref. 10 for a compilation). Worldwide structure databases such as the Protein Data Bank (PDB)[1] [11] have also been using Rasmol and Chime as viewers.

CHIME'S TWILIGHT

The birth of Chime was based on the plug-in architecture (complementary modules for the web browser) developed by Netscape. These plug-ins were later supported by Microsoft Internet Explorer, and MDL made several updates of Chime to allow a greater compatibility with this browser. Despite this, full compatibility was only assured for Netscape 3 or 4 under Windows and Macintosh operating systems. Under Mac OS X, only Netscape 4 in Mac Classic mode is compatible with Chime. In the Windows arena, modern Gecko-based browsers (such as Netscape 6 and later, Mozilla, and Firefox) are not supported by the Chime installer, although this can be tweaked by manually copying a file. The increasing pool of Linux systems has also been kept away from the chance to use Chime. Elsevier MDL has declared no plans to update the software to cope with these limitations, nor to release the source code to be developed by others.

In summary, the use of Chime as a plug-in has increasingly become a burden for web page designers, given the extensive user base of Internet Explorer under Windows, of modern browsers such as Mozilla and Firefox under any platform, and of Linux systems in both scientific and personal environments. The current state of the art in web page design, standards (HTML,[2] XHTML, and CSS), and technologies, as well as hardware resources, has also introduced the possibility of higher quality graphics and better interaction with content.

In the last few years, these limitations have induced the emergence of several alternative pieces of software for the inclusion of molecular models within web pages, mostly in the form of Java applets (to assure independency from operating system and browser). An excellent overview of many of these is available at Ref. 12, but we believe that Jmol is the most powerful, versatile, and promising one.

Jmol TO THE RESCUE

Jmol [13][3] is free software, an open source project in molecular visualization developed by a community of volunteers. It is available for free at www.jmol.org. Among the relevant features that make Jmol a promising tool to replace Chime and even expand its potential are:

- It is open source, meaning that anyone can get the source code and modify it. This warrants future development. The license is GNU Lesser General Public License [14].
- It is available freely via internet and at no cost.
- It is written in Java programming language [15], which makes it compatible with all operating systems.
- It is compatible with all major web browsers (all that support the Java plug-in or "Java Virtual Machine").
- It provides triple implementation: standalone application, applet for embedding in a web page, and development tool kit for inclusion into other Java software.

HISTORY OF Jmol

Jmol has evolved through several versions, led by successive developers. It began (circa 1999) as a replacement for XMol, a molecular viewing program developed at the Minnesota Supercomputer Center that was no longer maintained and whose source code was not available to users. Jmol was started by Dan Gezelter under the OpenScience project [16], which is dedicated to writing and releasing free and open source scientific software. Handled by successive developers, Jmol continued its progress under SourceForge [17], incorporating new features.

Around 2002, the possibility arose of improving Jmol, at that time on version 9, to make it a viable replacement for Chime. Under the leadership of Michael T. "Miguel" Howard, the graphics engine was rebuilt to be more efficient, allowing it to work with macromolecules; the Rasmol/Chime script interpreter was expanded; and new file formats were supported (also opening the means for easily adding future formats). This marked the birth of Jmol version 10, in the form of prereleases. During 2003 and 2004, several users around the world contributed to Jmol development by testing Jmol, explaining chemical concepts, and explaining the scripting behaviors of Rasmol and Chime, until the first official version, Jmol 10.00, was released in December 2004. From then on, development has continued, especially incorporating new functionalities that go beyond what can be achieved with Rasmol and its set of commands. As a result, version 10.2.0 has been recently released (April 2006), and more enhancements are on their way.

TECHNICAL SPECIFICATIONS FOR Jmol

Hardware Requirements—The hardware resources required by Jmol are moderate. Performance is a function of molecule size, window size, and image complexity. Due to engine redesign on version 10, a good three-dimensional graphics performance is achieved without the need for a specialized graphics card. Neither Java3D, OpenGL, nor hardware acceleration is used. More detailed technical information on software implementation is available at the Jmol website [13].

Software Requirements—Microsoft Windows, Mac OS X, and Linux operating systems are compatible with Jmol. A Java Virtual Machine (also known as *JVM* and sometimes *Java plug-in*), version 1.4 or later, must be installed.

In addition, to use the applet, Java must be active for the web browser used. The browser can be any recent one (as Miguel Howard puts it, "one from this century"), actually, any that supports Java; this includes, at least, Netscape 7 and 8, Internet Explorer 5.5 and 6.0, and

[1] The abbreviation used is: PDB, Protein Data Bank.

[2] See Appendix for acronyms and definitions of technical terms.

[3] Sources of detailed information about Jmol are its home page www.jmol.org, its mailing lists, the developers' and users' collaborative space wiki.jmol.org, and the documentation for scripts at www.stolaf.edu/people/hansonr/jmol/docs. The correct spelling is Jmol, not JMol, which is an unrelated program developed by Will York, from the Complex Carbohydrate Research Center, University of Georgia, Athens, GA.

TABLE I
Software requirements of Jmol as compared to Chime

Chime plug-in	Jmol applet
Limited compatibility.	Broad compatibility.
Must be installed in each computer and each web browser.	Cannot be installed, it is automatically downloaded with the web page. Java must be installed if not already included in the system (an easy process, guided from the web browser).
Very fast loading (as it resides in the user's computer).	Slower loading (must be downloaded each time from the web server; size of the applet files is close to 800 kb). The initial responses of Java and of Jmol are somewhat slow, then caching takes place and behavior is agile.
Requires configuration of the web server (for MIME[a] types).	No configuration of web server is needed.
Allows local use in the same conditions as from server.	Local use (*i.e.* running off hard disk or CD-ROM) needs precautions when the author programs the pages.

[a] MIME, multipurpose Internet mail extensions.

recent versions of Mozilla, Firefox, Safari, and Opera. For most web pages, that include controls to interact with the model in the applet, JavaScript must also be supported and active in the browser. Table I summarizes a comparison between Jmol applet and Chime regarding software requirements.

Jmol'S FEATURES FOR MOLECULAR VISUALIZATION

FILE FORMATS

Jmol, as is true for all molecular visualization software, uses molecular coordinates files for input. The most usual formats (pdb, mol, xyz, cif) are accepted, as well as others that are more specialized or restricted in their use. Among them are: ABINIT, ACES II, ADF (Amsterdam Density Functional), CIF/mmCIF, CML v2.0, CSF (Fujitsu CAChe Chemical Structure File), GAMESS, Gaussian, Gaussian Cube, Ghemical MM, HyperChem's HIN, Jaguar, MDL molfiles MOL and SDF (V2000 and V3000), Mopac, NWChem (Pacific Northwest National Laboratory), PDB, multi-PDB (from NMR), Q-Chem, SHELX (RES), Spartan, and XYZ (single and multiple frame). All of them can be either plain or compressed with the gzip algorithm. The format is recognized automatically upon reading the file, without giving any instructions. The program has been designed to be modular so as to be easily expanded into new formats since the file parser is independent of the core functionality.

In addition to reading molecules, Jmol can read script files, *i.e.* text files with instructions or commands to be applied to the model (*e.g.* rotation, translation, type of rendering, coloring, selection of part of the molecule to be acted upon, spinning, animation, etc.). Most Chime commands (inherited from Rasmol 2.6 as well as those specific to Chime) are accepted, and several new Jmol-only commands have been added.

Regarding output, although it is not the primary aim of this program, given its visualization nature, some options are available. The standalone application can export images (jpeg, png, ppm), POV-Ray files, and PDF files, whereas the applet can save the molecule file, in the original format in which it was read. Rasmol's ability to save script files, reproducing the current view and state of the model, is not included in Jmol, although it may be part of future versions.

MODEL RENDERING AND VISUALIZATION

Color—For historical reasons, Rasmol is limited to 8-bit color (*i.e.* a 256-color palette); Chime retained this limitation. This allows for reasonable but limited quality in the rendering of models. Jmol has overcome this constraint and uses full color, resulting in greatly enhanced quality of models (Fig. 1).

Text—Font quality has also been significantly improved over that available in Rasmol and Chime (Fig. 2). Further, font face (serif, sans serif, or monospaced), style (plain, italic, bold, or bold+italic), size, and color can be set separately for each text element. Atoms can be labeled with text, as in Rasmol and Chime. Text can also be placed within the program window on nine static positions (top, middle or bottom, and left, center or right).

Atoms—As in Rasmol/Chime, atom size can be controlled, from none (invisible) to space fill. Jmol accepts percentages of van der Waals radii as well as absolute size. Ionic radii are also supported, as an alternative to atomic ones. Dot spheres can be rendered, as in Rasmol.

Another novelty is the use of "stars" (a set of crosshairs), tetrahedra, or octahedra instead of spheres, which is useful for areas such as inorganic chemistry, crystallography, mineralogy, and materials science. (Stars are one of the additions in the Rasmol 2.7 series, absent from 2.6 and thus from Chime.)

Chemical element recognition has expanded from 28 elements using 15 colors (in Rasmol and Chime) to the full periodic table (109 elements and colors), each element receiving a unique color and its proper radius (see Ref. [18] for a demonstration). This, again, affords potential for diverse fields, such as inorganic and organometallic chemistry.

Atom color can be chosen among CPK and several common coloring patterns (by identity of amino acid, by secondary structure, by order in the polymer, by charge, and so forth). New in Jmol are the abilities to redefine an element's default color and to render partial transparency (not just for atoms, but bonds, schematic representations, and other objects).

Bonds—Bonds are rendered as cylinders, whose diameter can also be set, as in Rasmol (no innovations here).

Schematic Representations for Macromolecules—Of utmost importance for biological macromolecules is the

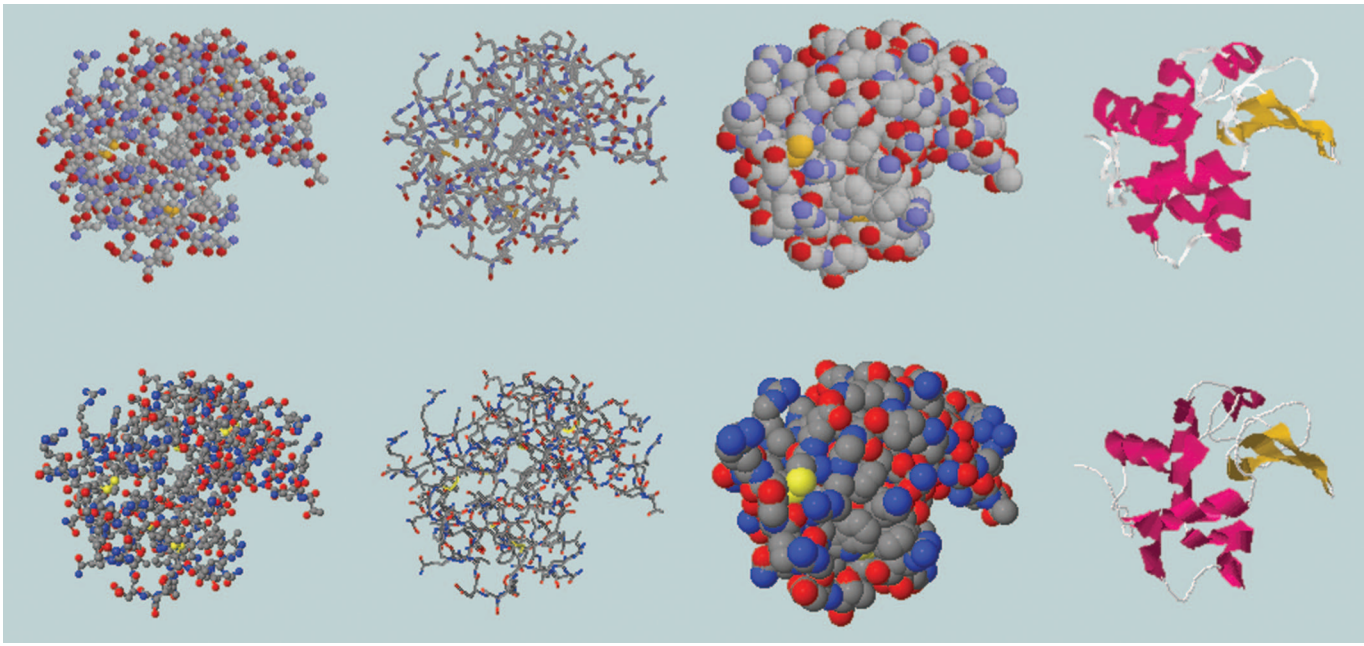

FIG. 1. **Renderings of a protein molecule by Chime (*top*) and Jmol (*bottom*).** From *left* to *right*, ball and stick, sticks, space fill (all three with CPK coloring), cartoons (with color by structure). The model is lysozyme, 1HEL.pdb

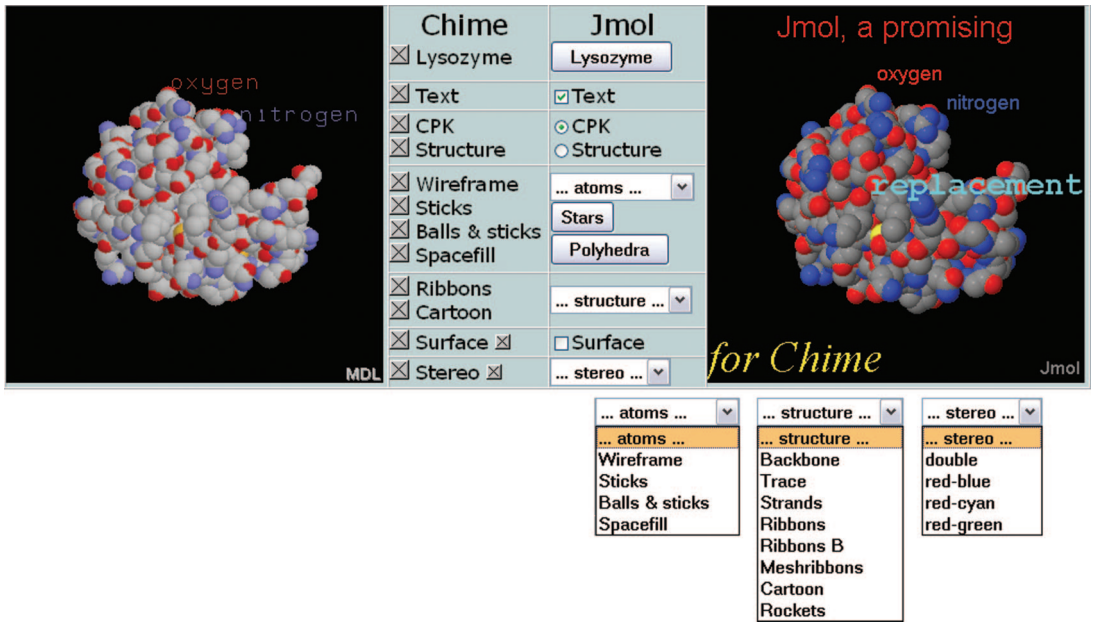

FIG. 2. **A comparison of rendering quality for atoms and text and of web page controls that allow interaction with the molecular model, for Chime (*left*) and Jmol (*right*).** Whereas Chime uses proprietary buttons, Jmol allows any form controls available in HTML: push buttons, checkboxes, radio buttons (all INPUT controls) and pull-down menus (SELECT controls), as well as text or image hyperlinks (not shown). The *lower part* shows the content of the opened pull-down menus. The controls and options shown are not standard for the programs but are written by the author of the web page. The model is lysozyme, 1HEL.pdb

ability to simplify the structure of the molecule instead of showing all its atoms and bonds. To renditions existing in Rasmol and Chime (backbone, trace, ribbons, strands, cartoons), Jmol adds ribbons with borders and wire mesh ribbons. Some differences exist in the rendering of cartoons, which have no thickness in Jmol; in compensation, solid planks and cylinders ("rockets") may be chosen for proteins. Nucleic acids (DNA and RNA are separately discriminated by Jmol) have a cartoon that shows bases as well as backbone.

Other Improvements

- Hydrogen atoms can be hidden and shown in any moment.
- A certain position of the model can be defined and can later be targeted from the current one using an automatically generated smooth movement of rotation, translation, and zoom.
- Zero-point (or orthogonal) perspective, the one used by Rasmol, can be exchanged for one-point (or con-

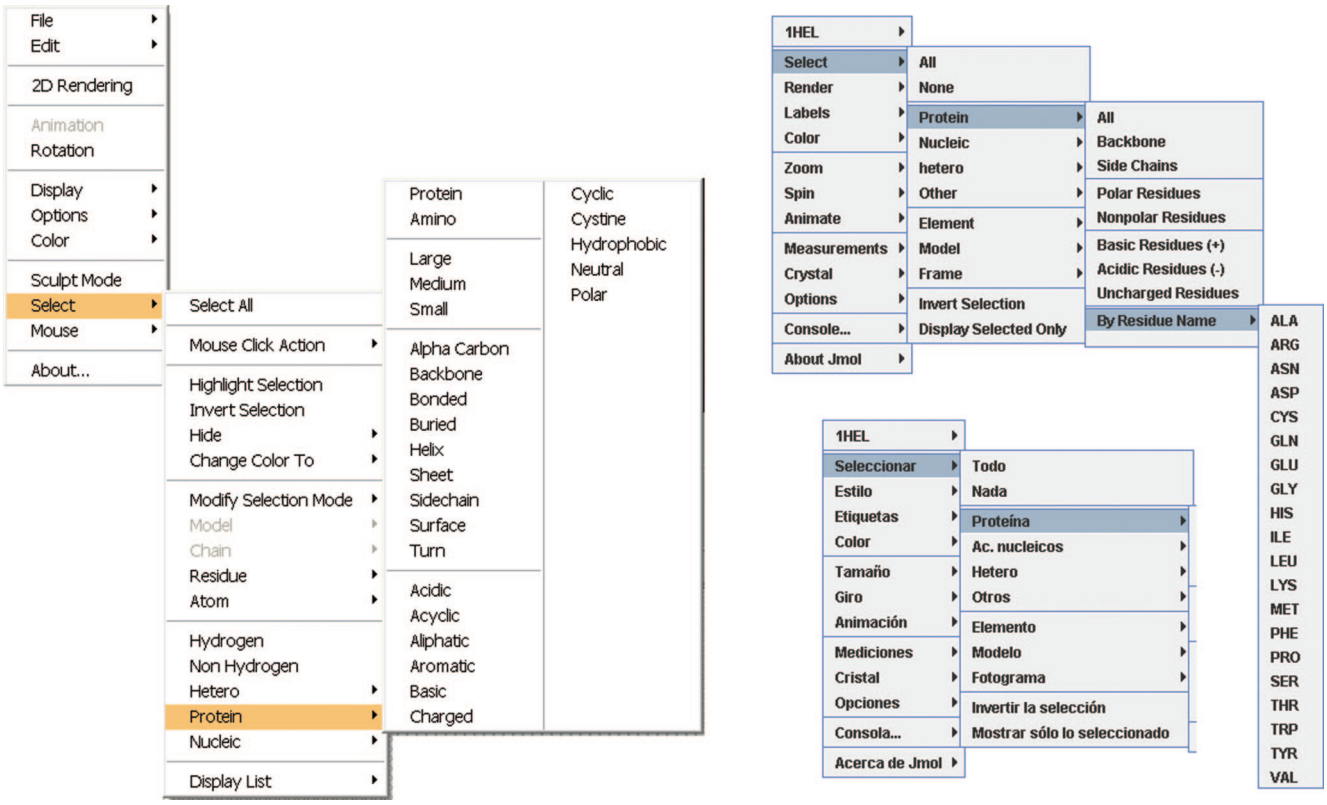

FIG. 3. **Example of the pop-up menus for Chime (*left*) and Jmol (*right*).** Despite somewhat different arrangement in submenus, overall functionality is equivalent in both programs. The Jmol menu has more options than Chime, which can make it more powerful but also more difficult for novices. The *lower left inset* on the Jmol menu illustrates a portion of the same in Spanish, to highlight that in Jmol, the interface language is automatically adopted depending on the user's operating system language.

ical) perspective, the default in Jmol, allowing a better perception of depth.

- Stereographic rendering includes Rasmol-like side-by-side stereo display and new anaglyphic rendering, suited for "three-dimensional glasses" using red+blue, red+cyan, or red+green lenses.
- More options are available for monitor lines and measures.
- The model can be sliced ("slab" effect) from the back as well as from the front (the only choice in Rasmol).
- Molecule vibration can be shown, if provided by the molecule file format (xyz, Gaussian).
- In addition to the pop-up menu (illustrated in Fig. 3), offering plentiful commands to act on the molecule rendering and measuring, a command-line window or console is available for the use of advanced instructions or during web page design. This is similar to the Rasmol command window, which is unavailable in Chime.
- Basic actions with the mouse (nowadays called *mouse gestures*) present in Rasmol and Chime are compatible with Jmol, but more diverse gestures have been added (for example, for taking measurements).
- For the web page author, a JavaScript library is provided (Jmol.js), allowing web page authors to easily create controls that interact with the model.

Molecular Surfaces—The use of surfaces replacing or covering the molecular model is of great advantage in illustrating the shape of proteins and interactions among them and with ligands. The surface simplifies the representation and gives a realistic perception of the protein's outline and volume, binding pockets, etc. This feature is one of the few points in which Jmol has not yet advanced to the point of replacing Chime.

Surface calculation was also lacking in Rasmol, but it was one of the few extensions added to Chime, allowing it to calculate solvent-accessible surfaces and render them in different colors and transparencies. The latest version of Rasmol, 2.7.3, has also added Lee-Richards surfaces, both solvent-accessible and solvent-excluded [5].

Chime can also load surface data contained in external files, in either pmesh or Gaussian formats. In this modality, Jmol is also proficient; it loads pmesh files and Gaussian Cube files, rendering *pmesh* surfaces and *isosurface* surfaces. These have found use, among others, in representing atomic and molecular orbitals.

INTERACTIVE MODELS, ACTING ON THE MOLECULAR MODEL FROM THE WEB PAGE

Chime incorporated the ability of changing the molecular model from within the web page, through commands either run when loading the page or invoked in response to user actions (in both cases, instructions are preprogrammed in the page source code by the web author). The functionality can be achieved via two systems: first, by using the parameters of the EMBED tag that inserts the model and the buttons acting on it, and second, by using the richer set of options that form Rasmol script language

(which are actually passed to the Script parameter of the EMBED tag).

Of these two approaches, Jmol has inherited the second, along with the script language. However, since the applet is written in Java, a different mechanism of communication is implemented. Usually, this involves JavaScript language invoked from the source code that builds the web page; JavaScript commands are coupled to hyperlinks, form controls, or even mouse actions over the page elements. This allows for a wider choice in the kind of controls, better integrated in the standard look-and-feel of the operating system, and a richer user experience of interaction. Fig. 2 illustrates this with an assortment of controls.

CURRENT DEPLOYMENT OF Jmol IN WEBSITES

As has been mentioned at the beginning of this article, for a number of years, Rasmol and Chime have been the viewers of choice in web portals to structure databases; best known among them is PDB [11]. This stresses the fact that molecular viewers are not mere educational tools but also remarkable resources for research, helping the understanding of macromolecule features and structure-function relationships. As the limitations in browser compatibility arose, institutions in charge of databases had to find a balance between directing users to register, get, and install Chime, even implying the installation of the uncommon and outdated Netscape 4 browser, or finding a new viewer compatible with the recent browsers. As a result, sooner or later, they had to implement or develop one of the Java viewers (reviewed in Ref. [12]). As a representative example, the new website for PDB at Research Collaboratory for Structural Bioinformatics (RCSB), starting January 2006 [11], has switched completely out of previous Chime and Chime-based tools (such as FirstGlance and ProteinExplorer) toward a choice among KiNG, Jmol, WebMol, Protein Workshop, and QuickPDB, all of them Java applets. OCA [19], another prominent portal for PDB data, offers Jmol, FirstGlance [20] (the new version, which is based on Jmol), AstexViewer, and RasMol (which actually becomes Chime if this is installed on the browser).

Educational web pages using Jmol are also flourishing, mostly by conversion of existing Chime sites, yet much remains to be done. As a modest contribution to this conversion process, let us reference my website [21] and the BioROM collaborative project [22] in which I participate.

CONCLUSION

Jmol is a free, open source program that can effectively be a substitute for Chime in developing educational web pages that are compatible across browsers and operating systems. It can also replace Rasmol for basic investigation of biomolecular structure and for deploying medium-to-advanced level activities for students. Display features are outstandingly adequate for biomolecules, both small and large, as well as for other fields such as crystallography, materials science, and organic and inorganic chemistry.

Acknowledgments—I express my gratitude to Prof. Eric Martz (University of Massachusetts), long-time advocate of molecular modeling teaching, provider of Rasmol and Chime information and support on his website, of teaching-oriented recommendations and sample materials, of the excellent Protein Explorer software for macromolecule visualization and analysis, and of other countless contributions, including the recent FirstGlance in Jmol. Appreciation is also due to Roger Sayle and MDL Elsevier for developing and offering Rasmol and Chime, respectively, to the world. Finally, I want to recognize the work of the Jmol v.10 developers team, Michael Howard, Egon Willighagen, Nicolas Vervelle, Bob Hanson, and others, offered for free to the benefit of the scientific and educational communities, and for including features that allow it to be the relay for Chime across diverse web browsers and operating systems.

APPENDIX

EXPLANATION OF ACRONYMS AND TERMS:

CPK = Corey, Pauling, Koltun

- A color scheme conventionally used by chemists, based upon the colors of the popular plastic space-filling models that were developed by Corey and Pauling and later improved by Koltun.

CSS = Cascading Style Sheets

- "A simple mechanism for adding style (*e.g.* fonts, colors, spacing) to Web documents." (Quoted from www.w3.org/Style/CSS.)
- "A stylesheet language used to describe the presentation of a document written in a markup language." (Quoted from Wikipedia.org.)

HTML = HyperText Markup Language

- "HTML is the *lingua franca* for publishing hypertext on the World Wide Web. It is a non-proprietary format based upon SGML, and can be created and processed by a wide range of tools, from simple plain text editors to sophisticated WYSIWYG authoring tools. HTML uses tags such as <h1> and </h1> to structure text into headings, paragraphs, lists, hypertext links etc." (Quoted from www.w3.org/MarkUp.)
- "A markup language designed for the creation of web pages with hypertext and other information to be displayed in a web browser." (Quoted from Wikipedia.org.)

Java

- (Java is a trademark of Sun Microsystems, Inc.)
- "A number of computer software products and specifications from Sun Microsystems that together provide a system for developing and deploying cross-platform applications." (Quoted from Wikipedia.org.)

JavaScript

- "The name of Netscape Communications Corporation's implementation of ECMAScript, a scripting programming language based on the concept of prototypes. The language is best known for its use in websites, but is also used to enable scripting access to objects embedded in other applications. Despite the name, JavaScript is only distantly related to the Java programming language." (Quoted from Wikipedia.org.)

XHTML = eXtensible HyperText Markup Language

- "A family of current and future document types and modules that reproduce, subset, and extend HTML 4. XHTML family document types are XML based, and ultimately are designed to work in conjunction with XML-based user agents." (Quoted from www.w3.org/TR/xhtml1.)
- "A markup language that has the same expressive possibilities as HTML, but a stricter syntax. XHTML is an application of XML, a more restrictive subset of SGML. It is a reformulation of HTML in XML." (Quoted from Wikipedia.org.)

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