The Virtual Museum of Minerals and Molecules: Molecular Visualization in a Virtual Hands-On Museum

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ABSTRACT

The Virtual Museum of Minerals and Molecules (VMMM) is a web-based resource presenting interactive, 3-D, research-grade molecular models of more than 150 minerals and molecules of interest to chemical, earth, plant, and environmental sciences. User interactivity with the 3-D display allows models to be rotated, zoomed, and specific regions of interest to be highlighted. The VMMM has been online since 1998 and currently serves 100,000 to 250,000 unique visitors annually from two mirror sites. In concept, it is a blend of a static bricks-and-mortar physical museum with wings, galleries, and displays with dynamic 3-D first-person video games. This museum is virtual not only in the sense that it exists in electronic format but also because the molecular size of the objects makes them colorless and imperceptibly small. To date, molecular visualization has been enabled in browsers using a proprietary third-party plug-in; compatibility with diverse platforms and browsers has been reduced over past years and recourse to open-source, molecular visualization Java applets may be required to avoid technological obsolescence.

The Virtual Museum of Minerals and Molecules (Barak and Nater, co-curators) is a web-based resource presenting interactive, 3-D, research-grade models of more than 150 minerals and molecules of interest to chemical, earth, plant, and environmental sciences. The Virtual Museum can be viewed online without fee, subscription, or password protection at the following two mirrored site URLs: www.soils.wisc.edu/virtual_museum/ or www.soils.umn.edu/virtual_museum/ (both verified 15 Apr. 2005). At present, requirements for viewing this work are commonly available browser software (Microsoft Internet Explorer [MSIE] 5.5+ or Netscape Communicator 4.7) and free browser plug-ins, principally Chime (both PC and Mac OS9 versions downloadable from MDL Information Systems, at www.mdlchime.com; verified 15 Apr. 2005) and any of a number of VRML plug-ins.

The objective of this article is to describe the central concept and design of the VMMM, its audience, the underlying technology and history of that technology, issues of funding and continuity, and future developments of the Virtual Museum.

CONCEPT AND DESIGN

Conceptually, The Virtual Museum of Minerals and Molecules is a blend of a physical “mortar-and-marble” museum with Wolfenstein 3-D (id Software, Mesquite, TX), one of the earliest (1992) first-person “3-D” computer video games and archetype of DOOM and QUAKE, games currently popular among college-age students. The advanced state of mineral classification (i.e., oxides, carbonates, silicates, etc.) readily fits the wings/galleries/rooms/displays hierarchal structure of physical museums (The Toledo Museum of Art and the Field Museum come to mind); even so, organic minerals and inorganic quasiminerals logically fall into the Minerals Wing. By contrast, the organization of the Organic Wing is more idiosyncratic—by choosing among the various natural, synthetic, small and macro- molecules, galleries were created organized around specific functional groupings, such as transmembrane proteins, pesticides and contaminants, and chelates. This organization of these materials was not obvious and necessary; others might have attempted to create tightly organized, linear tutorials out of the same materials. Instead, the exploration-based museum structure used here lends itself to informal learning as well as picking out individual items or clusters of items of interest. In addition to the categorical index, an accompanying alphabetical index allows for rapid access of a particular item.

The scope of the Virtual Museum encompasses minerals and molecules ranging from the familiar and crystalline (such as kaolinite and smectite; Fig. 1) to the newly discovered and biological (such as aquaporin and the potassium transport channel; Fig. 2). The typical VMMM webpage display for a mineral or molecule consists of three fundamental parts, with a navigation bar above: a frame with the 3-D model, a small frame that contains the element key and switches between display states, and a text frame containing text and clickable buttons. The computer-generated chemical model of the mineral or molecule of interest can be rotated, zoomed, and highlighted to reveal particular regions of interest. The element key frame identifies constituent atoms of the model by color and also contains a series of clickable buttons that switch the display state of the mineral or molecule between stick, ball-and-stick, space-filling mode, or ribbon/helix. The text frame contains contextual information about the history and science of the mineral or molecule, including reference to the primary literature from which the 3-D coordinates were drawn, and may contain electron micrographs and other appropriate instructional aids and materials, as well as references to the primary literature; the text frame also contains clickable buttons that interact with the 3-D model to highlight particular structural features of interest, such as silicate layers (Fig. 1b) or alpha helices (Fig. 2), particularly those that relate to function. For minerals, the text frame links to a webpage describing crystallographic space group, axes and angles, and atomic positions. Some displays employ animation scripts that flip, rotate, or highlight various features either on load or upon user mouse.
click; such animations (e.g., Fig. 3) can be used to smoothly move between one molecular visualization mode to another, while still permitting user interactivity with the model during the transition, in a manner that has no physical equivalent. The cumulative experience of the curators has been that construction of the 3-D content of the models themselves was relatively straightforward and routine compared with the more challenging task of identifying the key points and construct-
ing the scripts and highlighting features, a task for which no parallel quite exists for 2-D illustrations or static 3-D models.

Active learning is encouraged in the VMMM format through user interactions with displays. For all displays in the VMMM, click-and-drag mouse operations allow the minerals to be rotated and zoomed; mouse clicks on the buttons of the text frame allow predetermined features to be highlighted in the 3-D window, while clicks on the buttons in the atom key frame change chemical representation. Furthermore, the type of spatial “literacy” now required for “molecular 3-D literacy” has traditionally been reserved for artists, specifically sculptors, architects, and other 3-D professionals (S.M. Halpine, personal communication, 2003; artist-biochemist) and so there is reason to hope, if not expect, that these interactive 3-D materials will leave a subtle but substantial impact in the deep intuitive learning required for modern science education.

Although we felt challenged to use 3-D to bring as much attention to scientific materials as to entertainment, we are cognizant of the fact the entire current generation of experts in these minerals and molecules was trained in the absence of such highly visual, computer-implemented tools for either science or entertainment. The next generation of experts, however, will have grown up with these tools for entertainment and will require that the same 3-D visualizations carry over into their education to provide sufficient stimulation and time on task. Fortunately, innovations in web-based 3-D visualization are currently making their way through chemistry, organic chemistry, and biochemistry instruction (Mount, 1996; Shusterman and Shusterman, 1997). It is premature to attribute higher performance teaching and learning to the new materials that the VMMM and like sites offer. However, it is widely recognized that the traditional materials and the ways they are used do not promote active learning or exploration, both of which have been shown to significantly enhance comprehension and advanced knowledge acquisition (Spiro and Jehng, 1990; Najjar, 1996). Many studies have shown the value of interactive and active learning in education (Bosco, 1986; Fletcher, 1989, 1990). Stafford (1990), in an examination of 96 learning studies, showed that learning achievement and long-term retention of knowledge were positively associated with interactivity; Bosco (1986) and Fletcher (1989, 1990) found, in summaries of 75 learning studies, that interactivity enhanced both the rate at which people learn and their attitudes toward learning the material (Najjar, 1996).

It is noteworthy that the Virtual Museum of Minerals and Molecules is virtual not only in the sense that it exists only in electronic format but also because its contents often exist at a nanoscale penetrable only by X-rays, electron microscopy, and atomic force microscopy, and therefore cannot be meaningfully displayed as real objects under glass. Even when the symmetry of the display objects allows for larger substructures, for example, regular polyhedra centered on a central atom, protein tetramers organized as a cylinder, or layer silicates tesselating (semi)infinitely in all directions, those substructures are still incrustably small. Even the bright colors of the Virtual Museum displays are virtual because all its colored items, for example, atoms, exist at a size smaller than a single wavelength of any visible color and therefore the color of all displays is entirely a matter of convention and aesthetics.

**AUDIENCE**

Our Virtual Museum of Minerals and Molecules originated with lecture materials prepared for our own classes to illustrate a few molecules—chelates, ion transport channels, and a few minerals—and grew over the course of time to provide online lecture materials used in at least 20 undergraduate courses at our home institutions and elsewhere in the USA and the world. To the best of our knowledge, usage of the VMMM includes: (i) in-class use of individual displays by instructors using a computer and data projector; (ii) directed exercises in computer lab by students, including GeoWall stereoscopic 3-D projection; (iii) live links in web-based classnotes provided to students; and (iv) construction of polymer-based physical models using rapid prototyping machines based on the VMMM structural models. A recent Google (www.Google.com) search showed over 590 links to the Virtual Museum website, mainly from the “.edu” domain, mostly either instructors posting lecture notes with links or students using the Virtual Museum to construct class reports. Searches have additionally shown that VMMM materials have been used with attribution in peer-reviewed publications, online journals, patent applications, and internet newsgroups. Based on our weblogs, since going online in May 1998, the Virtual Museum has grown into a web-based resource serving between 100 000 to 250 000 visitors a year worldwide from its two mirrored sites, the large majority of whom come from outside the “.edu” domain and who likely participate in informal learning that fulfills the outreach mission of our state-funded universities to their state(s), nation, and world.

Aside from several presentations at professional meetings and word of mouth, publicity for VMMM has been largely
through internet search sites and their associated robot indexing agents, which often place VMMM displays on the first page of links returned for applicable keyword searches. Sites such as Google use proprietary algorithms, believed to be based largely on the quality of linking sites to rank sites for this purpose; a recently posted display on the biogenic mineral struvite was placed in the top 10 Google references (of 9500 on file) within one month of its posting. The Virtual Museum website is often placed on custom lists of web-based resources, such as “K12 at the UW-Madison, Educational Resources for Teachers, Students, and Parents” and the San Diego Super Computer Center.

Along the way, this emphasis on undergraduate education led to the award of the prestigious EduCause Medal (1999) for successful demonstration of the effective use of emerging learning technologies in undergraduate education, as well as recognition from leaders of our professional societies, who wrote to the department chair at the University of Wisconsin-Madison that the Virtual Museum is “…a jewel of the worldwide-web as it combines information, technology and artistry in a form with few equals,” “…one of the most innovative teaching tools I have seen,” and “…helping to educate and inspire the next generation…”

The editors of Scientific American selected the Virtual Museum as one of the top 50 scientific websites of 2003 and it was the “Site of the Week” selection of American Scientist online (www.americanscientist.org; verified 15 Apr. 2005) for 26 Oct 2004.

TECHNOLOGY

If the “mortar-and-marble” museums have foundations built on bedrock, the foundations of virtual museums rest on the shifting sands of time and technology. The Virtual Museum of Minerals and Molecules consists of a slowly evolving set of content files for chemical structures on web servers and a more rapidly changing set of implementations that make that content visible on the user/visitor’s client machine. The chemical files that contain the content of the display are, at their simplest (e.g., xyz format), lists of atom by element and x-y-z positions in space, leaving the work of calculating bonding of individual atoms to the visualization software to complete; more complicated files types include chemical bond information (.mol) and/or amino acid designation of the constituent acids (.pdb), if appropriate. File sizes depend on chemical complexity, of course, but range from 6 to 500 kb; files may be compressed for transmission using the gzip protocol.

The antecedents of the VMMM go back to RasMol, which was developed in the early 1990s as an open source, stand-alone viewer for these chemical file formats and which was ported to a number of operating systems, including Windows and Mac. In 1995, MDL used RasMol code as the core for the Chime browser plug-in for Netscape Communicator and MSIE. When the VMMM first went online in 1998, the browser mixture was evenly split between Netscape and MSIE, and both browsers were functional on computers with Windows and Mac operating systems. In retrospect, this appears to have been a ‘golden age’ of personal computing, with multiple interoperable and compatible choices of hardware and software. By 2003, MDL had shed support for any but Netscape v. 4.7x (now quite archaic since Netscape evolved to v. 7, and weakened along the way by competition with MSIE, then acquired by AOL, which subsequently chose MSIE as their browser of choice for its namesake web portal) and MSIE (which dropped support for Macintosh operating systems with OSX and is intended to become exclusively wrapped into the Windows operating system rather than remain an add-on).

The MDL’s efforts in Chime development have, since the gradual departure of most of the original team that assembled Chime, largely been limited to making minor bug fixes and updating the installation utility to correctly find and install with the user’s MSIE browser; development efforts have been shed for all but MSIE on the Windows operating system, even though individuals have been able to jackknife installations of Chime into Netscape v. 7 and Mozilla (an open source spin-off of Netscape). Currently, at Chime v. 2.6 SP5, no new chemical features of consequence have been added to Chime in 5 years, though many opportunities have presented themselves. The commitment of any commercial enterprise, even if well capitalized (MDL is now owned by Elsevier), to producing a browser plug-in that serves as a viewer for proprietary files must be conditional.

Fortunately, open source solutions are in the works to rescue not only VMMM but also other molecular visualization endeavors. RasMol has continued development as an open-source, stand-alone viewer and Jmol v. 10 has suddenly appeared as a command-for-command Chime substitute, both stand-alone and plug-in, but implemented using Sun Microsystems’ Java language, which is largely interplatform. Further, once the Java plug-in is installed in whichever platform and browser, the Jmol applet does not require user installation of a plug-in. This is not as obvious a plus as it might seem, since a 3-MB downloaded Jmol applet in browser cache is required in place of a similarly sized plug-in in the plug-in directory of the browser; a browser plug-in is ‘stickier’ than the applet since the applet will be purged when the browser attempts to find more space or when the user does so for privacy purposes, and will have to be downloaded again for next use. On the other hand, the applet will automatically update whenever the server indicates the presence of a newer version, which permits rapid and silent deployment of upgrades to the client. Even so, the use of the Jmol applet favors a broadband connection not implicit in the use of Chime.

FUNDING AND CONTINUATION

The university setting is conducive as a seedbed for developing educational and scientific projects such as the VMMM, particularly since the self-tasking nature of faculty positions encourages high-risk experimentation if reasonable expectation of recognition and reward is present. The prototype Virtual Museum was first publicly demonstrated at an impromptu seminar at a peer institution, providing important early encouragement to continue development. Early institutional support from both the University of Wisconsin and University of Minnesota on an internal competitive basis was crucial. A grant by a federal agency in 1998 paid for students and staff to bring the museum to about 150 exhibits over the course of 5 years.

Development costs aside, maintenance expenses of the VMMM are fairly minimal. At both the University of Wis-
consin–Madison and the University of Minnesota, the VMMM is located on a web server maintained by the academic departments, for which the marginal operating cost is negligible. Content is the responsibility of the curators but the server activities, including operating system updates and security, are the responsibility of departmental computer system administrators who handle all of the departmental server activities, including cpu replacement. Ethernet connection fees at the University of Wisconsin are paid by a combination of base support derived from grant overhead (variably 18–45% of direct costs, depending on agency) and a per capita charge levied by campus administration on colleges, departments, and administrative units without regard to bandwidth consumed by their activities.

Given that the bulk of the VMMM audience is external and that development costs are relatively high, external grants are essential and it is therefore instructional to consider how projects such as the VMMM fare in the current grant review process. Although the VMMM exists in online, interactive 3-D format, the current paper or pdf-to-paper grant proposal format does not show off the strengths of the approach. For example, a recent proposal for expanding and improving the Virtual Museum was discussed by 27 panelists and presented to the panel by two of the panelists, without any of the group actually viewing the online VMMM. Although written descriptions of the VMMM may be mixed with screen shots that look like high-end book illustrations, the static format neither distinguishes between true computer-implemented 3-D and simple 3-D shading, nor between full user-based interactivity with the display and preprogrammed flash-type animation or hypertexting. This difficulty is systemic—a program manager candidly stated that “(u)nfortunately, in fairness to all applicants, the review process cannot mandate reviewers look outside the page-limit restrictions imposed by the proposal submission guidelines…” Almost certainly, interactive 3-D digital museums of all sorts are therefore at a disadvantage in the conventional static, 2-D proposal process of funding, and alternative review procedures for interactive 3-D projects are desirable. Dynamic demonstrations of proposals and prototypes are more appropriate for this type of endeavor and are more likely to recognize the strengths and weaknesses of the VMMM and other virtual museums.

**FUTURE**

A 3-year grant from the USDA Higher Education Challenge program, started in late 2004, is assisting the transition of the VMMM into the next technological phase. The entire contents of the current VMMM are being converted into a database of eXtensible Markup Language (XML) files, to be regenerated using standardized eXtensible Stylesheet Transformations (XLST) into HTML code that is more easily modified across the entire site in the future. To avoid technological obsolescence, the VMMM is migrating to Jmol (described above) to restore the cross-platform, cross-browser performance that existed in 1998, but without the requirement that the user install a plug-in.

The VMMM is also fortunate in having Dr. Cynthia Stiles of the Department of Soil Science at the University of Wisconsin–Madison join the other two curators to help develop new content for the VMMM and a group of colleagues has agreed to assist as evaluators. In the near future, the VMMM will explore animations of processes such as diffusion, sorption, and ion exchange that animate the structures into function. As an addition to the current self-exploration mode, interpretative virtual “walking tours” will be added to allow guided tours through the museum displays to illustrate specific lessons in symmetry, atomic radii, coordination number, and so forth. Finally, with the innovations currently underway in the VMMM development, the near future promises the prospect of VMMM displays rendered in stereoscopic 3-D and “floating” off computer screens to exhilarate and inspire the next generation of science students.

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**REFERENCES**

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