Resources and Strategies for Creating Molecular Animations

Jerry E. Honts, Ph.D., Department of Biology, Drake University, Des Moines, IA 50311

Why create molecular animations?

Molecular animations have been used extensively in undergraduate science courses to teach concepts that are difficult or impossible to represent with static diagrams. Animations can assist learning by providing multiple perspectives of complex structures, or they can be useful in depicting changes in a system over time.

While some instructors create animations for their courses, many rely on animations provided by textbook publishers, supplied on physical media (CDs or DVDs) or deployed on the web. Even though there are numerous existing animations, some instructors will want to create new animations to assist their specific aspects of their teaching. Many instructors are intimidated by the complexity of the software used to create the animations found in textbooks and on the internet, many of which were created by artists with expertise in the digital realm. But with a little persistence, it is possible for any would-be animator to create simple and reasonably effective animations to communicate key ideas for which static figures are inadequate.

Animations can take on many forms, from simple frame-by-frame 2D animations, to complex cinematic quality 3D animations. While the latter receive the most attention, there is no strong evidence that their "realism" necessarily helps students grasp complex concepts (Smallman & St. John, 2005). An individual should weigh the cost (time and effort) required to create an animation versus the learning gains that are desired.

Strategies for making molecular animations.

There are two major strategies for making animations of molecules. The simplest route, which may be the easiest, is to record images that are dynamically generated from molecular graphics programs, such as many of the research level programs such as UCSF Chimera [see tables for web links]. The recorded movies can be subsequently edited and annotated in one of many video-editing programs (such as Adobe Premiere or Apple FinalCut-both of which have simpler, cheaper prosumer versions). High quality movies can be quickly rendered using the powerful graphics engines underlying these software packages. The downside, however, is that the choreography of events is somewhat limited. Some of this can be made up by multiple "shots" and post-recording editing. Many of these programs also have a limited ability to "morph" between different molecular conformations, something that can be quite useful in depicting the conformational changes of macromolecules such as proteins. Extensions to these programs (such as the eMovie plug-in in PyMol) can be of considerable assistance in the creation of animations.

These research-level molecular graphics programs are also able to import data from programs that simulate molecular dynamics, by reading in data files that describe the trajectory of atoms or molecules over time. The advantage is that these molecular graphics programs can provide a much more elaborate rendering of the molecules in motion, since they can vary the form and shading the molecular representations, as well as spotlights, shadows, and depth cues.

UCSF Chimera http://www.cgl.ucsf.edu/chimera/	pre-installed Movie
UIUC VMD http://www.ks.uiuc.edu/Research/vmd/	pre-installed Movie extension
Schrödinger (DeLano) PyMol www.pymol.org/	pre-installed extension also: eMovie plug-in http://www.weizmann.ac.il/ISPC/eMovie.html

The more difficult path is to create these animations from scratch in a dedicated animation program. There is no royal road to geometry, and likewise is no easy path to the creation of more complex molecular animations. Most of the major applications have a formidable learning curve for creating anything beyond translation, rotation, and scaling of objects. But this is not a reason to avoid such efforts, since with a couple of weeks of hard work, the basics can be mastered, and much more complex animations can be created. Manuals can be useful, but there are also quite a number of online sources for instruction. Notably www.lynda.com or www.digitaltutors.com provides exceptional training for a reasonable fee for most of the programs described below. These online training libraries wonderfully illustrate the utility of animation, in that watching an instructor manipulate the program to achieve specific outcomes is accomplished in a way that is difficult to get from the printed page.

Good animations may not always be strictly literal. There are insights from artists, including those that created the first cartoons. A number of excellent books summarize these principles. While these insights may not be necessary in creating the simplest animations, they do have utility as the animations grow more complex.

Storyboarding is a necessity as animations grow more complex. It is best to first figure out exactly what you want to show, sketch it out via a storyboard, and only then begin the process of creating an animation. The storyboard can be a useful tool in helping the animator make critical decisions about what they should show versus what can be excluded.

Tools for creating molecular animations.

The actual mechanics of creating animations in dedicated software program requires a few things: (1) understanding how to use the basic drawing tools, (2) understanding how to use the tools that can transform the graphic objects, and (3) understanding how these transformations can be achieved over time. Most of these programs use a timeline metaphor for choreographing the changes over time. Use of this timeline requires an understanding of the concept of setting key frames, and letting the program help in the transformations of object that occur between those key frames.

The world is flat.

2D animations are intrinsically easier to create, but many of the basic principles can be extended to 3D animations. The preeminent tool for creating 2D animations is Adobe Flash, which renders animations in the SWF format that can with the use of the Adobe Flash player, be rendered in web pages. The majority of animations seen on the web have been generated in this manner. It does have the advantage that the Player is installed on the majority of personal computers, regardless of which operating system or browser is installed. This is likely to remain the default for some time, but there is rapid movement to using an open web standard, HTML5. Quite impressive animations can be achieved with HTML5, but the tools for creating these animations are still rather limited. But with the support of Apple and Microsoft, HTML5 is likely to become a major player in the next few years. At a recent developers' conference, Adobe demonstrated a Flash-to-HTML5 translation utility (reviews.cnet.com/8301-13727_7-20021213-263.html), suggesting that the adoption of this new standard will be rapid.

Adobe Flash http://www.adobe.com/products/flash/
SWISH Max http://anime.smithmicro.com/index_pro.php
Anime Studio http://anime.smithmicro.com/index_pro.php

One of the most useful additions to these programs has been the introduction of inverse kinematics, which is a way of animating jointed object with pivot points. While this might seem to be more relevant to character animation than molecular animation, these animating tools make animation of complex movements in molecules considerably easier, from changes in bond geometry to conformational changes in biological molecules, the ability to add "bones" to objects that constrain movements is a timesaver. In addition, some of these programs now have a simple physics engine that enables the simulation of some simple dynamic behaviors such as responding to collisions. The only other way to achieve this sort of physics is through programming scripts associated with the individual objects, such as ActionScript in Flash.

A bridge to the third dimension.

Some of these animation programs are able convey a limited representation of the third dimension, a sort of 2.5D perspective. Most of these programs accomplish this effect by placing 2D animations within planes that are stacked in the third dimension. Many contemporary cartoons use this strategy, and it can be effective in representing the third dimension on the cheap.

Anime Studio http://anime.smithmicro.com/index_pro.php
Toon Boom Studio and Toon Boom Animate http://www.toonboom.com/main/ http://www.toonboom.com/products/animate/

Molecular visualization programs and movie creation

Many animations strive to achieve a "realistic" three-dimensional effect, which can be accomplished as described above, but beyond simple translation, rotation, and scaling, things become much more complex or essentially impossible to do. At this point, it is necessary to make the leap to 3D modeling and animation programs. The effective use of these programs requires several distinct tasks: creating a 3D model of a molecular object, positioning it in a scene with respect to other objects, and then choreographing the relative motions of the objects, either as the individual objects change shape or orientation. or as they move relative to one another. These movements are usually orchestrated at the level of the timeline, which is fundamentally the same as in 2D animation programs, with the notable exception that many more parameters are being keyed over time.

There are many high-end 3D graphics and modeling programs that are used for this purpose. Most of these would be completely unaffordable if the software publishers did not provide huge discounts to academic users. The same software packages used by Pixar and in movies like Avatar can be purchased for less than $400, which provides a permanent license to faculty and students for non-profit uses. Many of the most sophisticated animations have been created in Autodesk's Maya program, but there are quite of number of other software packages that can yield high-quality animations. Maya, Cinema4D, and other software packages also include physics engines which can be of use in creating more physically realistic movements of molecules. Maya has been available for some time, but there are other programs that yield similar high quality "photorealistic" animations.

Another advantage that these high-end 3D graphics programs have is that they are both scriptable and extensible, and programmers have created interfaces to facilitate the creation of molecular objects and animating them. This has been especially true for Maya and Cinema4D.

There is also one open source "free" program, Blender, which has continued to evolve to gain the feature set found in the high-end 3D programs. While there may be more formal support for Maya and other commercial programs, there are excellent online resources and support forums for the Blender program. Since Blender is open source, it likely that interfaces will eventually be added via plug-ins that will enable it to directly import molecular structure data to create geometric objects.

Blender	http://www.blender.org/
Autodesk	Maya (part of a Autodesk Education Suite for Entertainment Creation) http://usa.autodesk.com/
Maxon Cinema4D	http://www.maxon.net/
Pixologic Zbrush	http://www.pixologic.com/home.php
Luxology Modo	http://www.luxology.com/
Side Effects Houdini	http://www.sidefx.com/
Cheetah3D	http://www.cheetah3d.com/
Unity3D	http://unity3d.com/

The first task in the 3D animation process is to create geometric models for specific molecular objects. This can be done by modifying primitive geometric objects, but is some cases it is possible to use molecular graphics programs to do the conversion of a structural model (such as a .pdb or .xyz data file) into a 3D modeling object format (such as .obj, .dxf, or .vrml). In this case, the converted models can then be directly imported into the 3D modeling program for further refinement and animation.

The individual molecular objects are then arranged on the "stage" within a viewing window, within the view of a specific camera that will capture and render this scene. Cameras, like the individual objects, can also be moved within the scene over time (dolly, pan, etc. as in cinematography). This is where the storyboard is essential in helping an animator make decisions of what will be shown and when. The movements of objects and cameras are choreographed via a timeline by setting keyframes and having the program generate the in-between frames of a movie. These programs have the ability to render animations in formats that can then be further edited in programs such as Adobe Photoshop or AfterEffects.

An alternative that needs more attention is to use snapshots of these animations to create a graphical narrative describing a mechanism or complex process. Given the familiarity of students and instructors with graphical narratives of all kinds (comics, graphic novels, anime), it is possible for an animator to tell a story using what could be considered a sparse form of animation. Readers understand the conventions for space and time used in these graphical narratives, and as a result, many of the actually movements can be obtained for free in the viewer's brain, since no one needs to see Superman, e.g., move in a step-by-step manner as he flies from point A to point B in Metropolis. In a sense, 3D is obtained for free.

Interactivity represents an additional level of engagement. Students are well-versed in 3D environments for gaming, and there are well-established pathways to bring 3D animations into interactive 3D environments, many of which have sophisticated physics engines that can automatically handle the dynamics of attraction, repulsion, and collisions. It is likely that there will be an increasing emphasis on deploying these sort of interactive environments on mobile devices such as Android or Apple iPhone. Some software packages are designed to facilitate this process, such as the Unity3D game development tool.

Another option for providing interactivity is through the use of sophisticated PDF (Portable Document Format) documents that incorporate interactive 3D images, with limited options for animation. These document can be created by Adobe Acrobat Pro and other programs from data created in 3D modeling programs. While this variation on the PDF document is used mostly in conjunction with CAD (computer-aided design) for engineering and architecture, there has been also some use of this interactive PDF format in journals such as Nature.

Once an animation is created, it is very important to get feedback from colleagues and students concerning its clarity and usefulness. It is typical that an animation will go through multiple rounds of revision before it is ready for use in the classroom.

How to use animations in the classroom?

Molecular animations can be used in a variety of ways in the chemistry or biology classroom. In many cases, they are used occasionally to highlight a specific point in a lecture setting that is difficult to relate with a static diagram or series of diagrams. A good example would be an animation that demonstrates a cyclic process, such as the pumping of sodium and potassium ions by the sodium-potassium ATPase in the plasma membrane of cells. Some courses and textbooks use animations extensively to teach chemical concepts, with a comprehensive set of animations that are linked to specific classroom exercises. In all cases, there should be a clear need for the animation to help students understand a concept. There are many cases in which an animation may not be necessary, and that a static diagram or written description is more effective. Animations, no matter how pretty, should support the learning objectives for the student.

There are challenges in effectively using molecular animations. First of all, to what degree do they communicate the essential point. It is quite possible to create an animation that prompts a "gee-whiz-this-is-neat" response from students without actually effecting much in the way of insight to the phenomenon that is being represented. The instructor can improve the delivery by showing the animations multiple times, with and without comments, and then followed up with questions for the students.

Another avenue for the use of animation in the science classroom is to have students create their own animations of a sort. Given that the animation programs have a steep learning curve, a simpler and accessible approach is to have the students create a visual or graphical narrative describing a complex structure or process. Creating storyboards of the type used to plan animations can be very effective in getting students to confront the essential aspects of chemical or biological processes because they are forced to explain the concept with their own words and pictures as they create a story that explains the concept to others.

Finally, assessment should have an important role in the use of animations. This can be done informally through course evaluations and review of test results, but whenever possible, there are advantages to setting up more rigorous tests of the efficacy of the animations in effecting learning. A number of studies have been carried out to look at the effectiveness of using molecular animations to teach chemical and biological concepts, but there is much more work that can be done to test various principles of design that make for a demonstrably effective learning tool.

References and Further Reading

Bromberg S, Chiu W, Ferrin TE. Workshop on molecular animation. *Structure*. 2010. 18(10):1261-5.

Iwasa JH. Animating the model figure. *Trends Cell Biol.* 2010 Sep 8. [Epub ahead of print]

McClean P, Johnson C, Rogers R, Daniels L, Reber J, Slator BM, Terpstra J, White A. Molecular and cellular biology animations: development and impact on student learning. *Cell Biol Educ.* 2005. 4(2):169-79.

McGill G. Molecular movies... coming to a lecture near you. *Cell*. 2008. 133(7):1127-32.

O'Day DH. The value of animations in biology teaching: a study of long-term memory retention. *CBE Life Sci Educ.* 2007. 6(3):217-23.

Smallman, H.S. & St. John, M., Naïve Realism: Misplaced Faith in Realistic Displays. 2005. *Ergonomics in Design* 13(3), 6-13.

Stith BJ. Use of animation in teaching cell biology. *Cell Biol Educ.* 2004. 3(3):181-8.

Return to Fall 2010 CCCE Newsletter