Molecular Dynamics in Education

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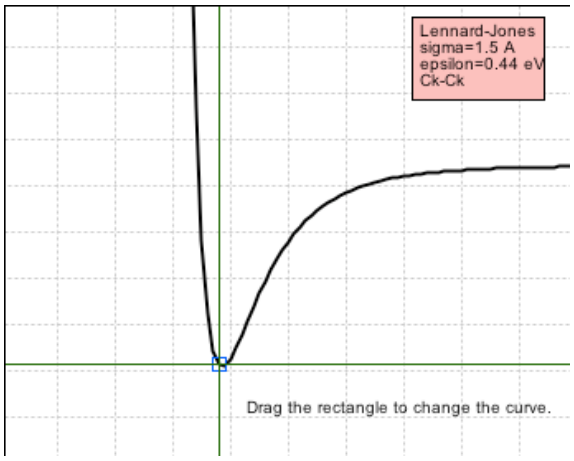
OVERVIEW

The Molecular Workbench is a modeling and authoring environment that can be used to explore a very wide range of atomic-scale phenomena that are important in biology, chemistry, and physics. The Molecular Workbench engine can be embedded in two different platforms for authoring and deployment in educational settings. Molecular Workbench software is free, open source software and a database of over 200 educational applications is available online.

The Molecular Workbench core model is an open source Java application that runs under Mac OSX, Windows, and Linux. It can be launched directly using Java Webstart. MW is smart enough to cache models locally, so once a model has been loaded from a server, it can be launched without connection to the server. You can even pre-cache all the models on a server, so the Molecular Workbench can work where connectivity is intermittent.

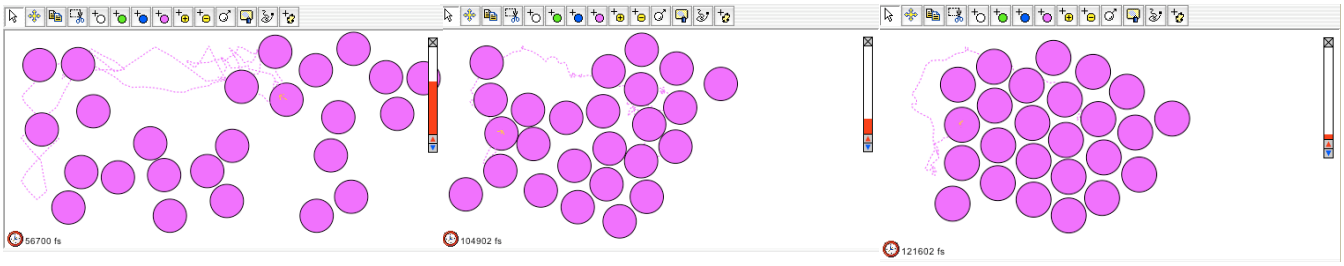
The Physics

Molecular dynamics is based on calculating the motion of atoms and molecules that obey Newton's Laws and various electrostatic forces that are important at the atomic scale. The basic force is the so-called van der Waals force, an attractive short-range force that occurs between all atoms. This force originates with the statistical fluctuations in the electric field produced by one atom that induce attractive dipole electric fields in any nearby atom.

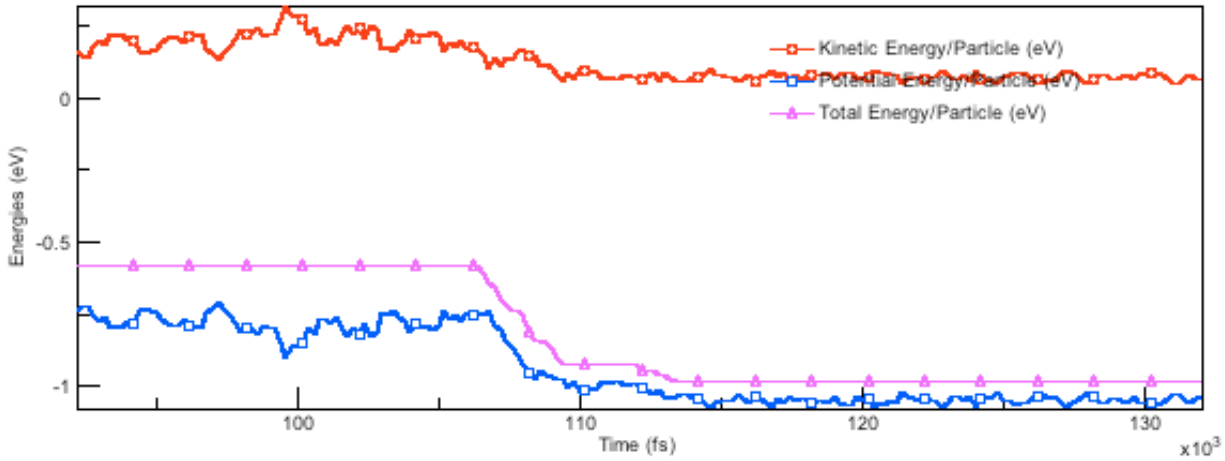


The Molecular Workbench uses a Lennard-Jones potential to approximate the van der Waals force and the strong repulsion between atoms. The potential is illustrated at right, which shows the L-J potential as a function of the separation of two identical atoms. In MW, the minimum can be dragged up and down to change the attractiveness of an atom, and left and right to change its effective diameter.

MW can calculate the motion of a large number of these atoms. If the atoms have a lot of kinetic energy, they form a gas. Remove some of the kinetic energy and they condense into a liquid. Remove more and they form a crystalline solid. The three snapshots below from MW show these three states of matter. The bar on the right of each snapshot shows the average kinetic energy (temperature) of the particles.

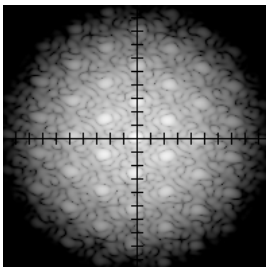


The graph on the next page shows the average kinetic energy (top), potential energy (bottom), and total energy (middle) of this system as kinetic energy was removed to make the change from liquid to solid. The first thing to note is that the middle line is flat most of the time. This is because the model conserves energy between times that the user interacted with the system by reducing the kinetic energy. The calculated potential and kinetic energies were highly variable, but their sums always stay the same between user interactions. This is powerful demonstration of the accuracy of the model, since there are millions of calculations involved, each one involving computing the Lennard-Jones potential for each atom and the force that it exerts on all nearby atoms.



Another important result can be seen in this graph as the user removed kinetic energy between 106 and 114 nanoseconds. The "cool" control that can be used to extract energy from the system slows down every particle by some percentage of its speed. You can verify that energy was removed because the center line, representing the total energy of the system, decreased. The graph shows that the kinetic energy dropped less than the potential energy. This appears surprising, since kinetic, not potential, energy was removed in the cooling process. The explanation is that by reducing kinetic energy, the atoms were able to move closer to each other, getting further down into the potential energy valley in the Lennard-Jones potentials. This converted the drop of kinetic energy into a larger drop of potential energy.

Since the average kinetic energy of a system is its temperature, this shows that the user removed energy as this system went from liquid to solid, but the temperature hardly changed. This is the physical origin of latent heat: the release of potential energy during a phase transition at a constant temperature. It is possible to set up a MW system that has no temperature change during gas-liquid and liquid-solid transitions.



Some Applications of Molecular Dynamics

To aid exploration, there are many tools available. The user can trace the motion of one atom, tag a group, replay a model like a videotape backwards and forwards, view the velocity of, or forces on, each atom, view the average density or speed of atoms, put barriers into the model, change its boundary conditions, and much more. The user can add charge to atoms to make ionic crystals. The illustration at right is an x-ray of the structure of the third model above.

In this section, the capacity of the Molecular Dynamics software is briefly described.

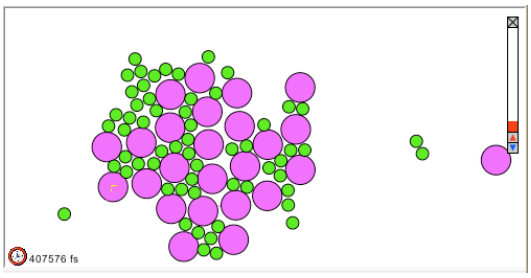
Using these tools, here are some of the possible explorations that students can undertake:

Diffusion. Students can investigate how quickly atoms can diffuse and see whether their size or mass affects diffusion rates. Users can measure the time required for one atom to reach the opposite edge. This is a chaotic system so even very small changes in starting position will make a huge change in the result. It is possible, however, to compute average time and this can be influenced by mass.

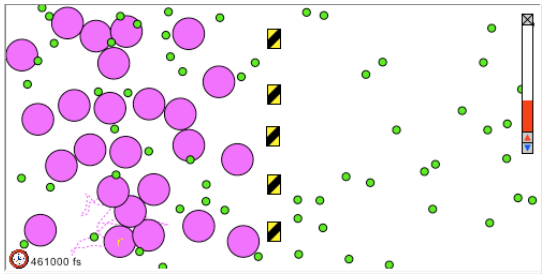
Crystal faults and annealing. If a user creates a solid crystal of many atoms by quickly cooling from a gas, it is possible to generate imperfect crystals: regions with different alignments, holes, and various faults. To increase imperfections, impurities can be added to the initial gas. If the crystal is heated near its melting temperature, these imperfections can work their way out, illustrating the molecular basis of annealing.

Entropy. Students enjoy playing a game that involves trying to preserve any regular arrangement of positions or speeds. No matter how a system starts, it always becomes more random, illustrating entropy increase. The system can be run backwards and the system appears random most of the time, but then it suddenly generates an unexpectedly low entropy configuration, the initial configuration.

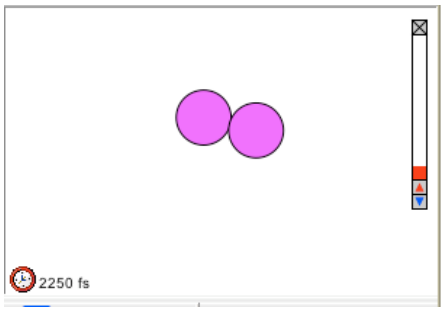
Gas absorption on solids. By using two kinds of atoms with different masses and Lennard-Jones potentials, the student can create a gas and a solid in the same model at the same time. Under most conditions, the most of the gas will absorb onto the surface of the solid. This is how separation columns, carbon filters, and xeolites work. If the gas is made of small atoms, they can interpenetrate the solid as shown at right. This is what hydrogen does to metals. This effect is exploited in metal hydride batteries, where hydrogen is needed but not as a gas, which could explode. On the other hand, this shows graphically how hydrogen can degrade a metal, a big problem in rocket design and in the coming hydrogen economy.

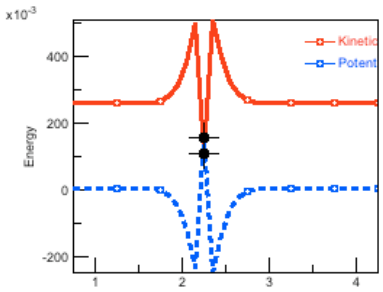


Osmosis. This confusing phenomenon is obvious when students make a barrier that only some atoms can get through. At right is a model of gas-phase osmosis created by placing rectangular barriers down the middle of the model and starting both big and small atoms on the left side. After running for a while, it is obvious that the density of small atoms is the same on both sides but that the pressure will be greater on the left because of all the big atoms there.

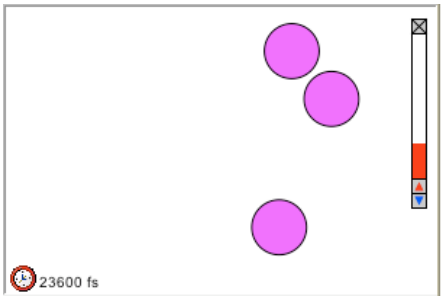


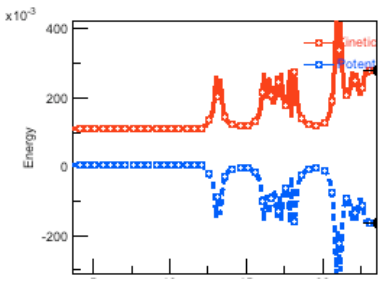
Two atoms. There is a lot to learn from the careful observation of just two atoms. Here two atoms collided and then sprang apart. The record was re-wound to the point when they were closest, indicated by the dot and crosshairs on the graph. Note how the kinetic and potential energies mirror each other. As they approached, they speeded up and, as a result, kinetic energy suddenly shot up at the expense of potential energy. But this did not last, because when their hard cores started overlapping, they repelled and the kinetic energy dropped as potential energy was stored in compression. Then they stopped, turned around and repeated the pattern as they flew apart. Students can learn about energy conservation by trying to get atoms to collide and "stick." Because of the way this system conserves energy, there is no way to get them to stay together if they start far apart and "fall" together.



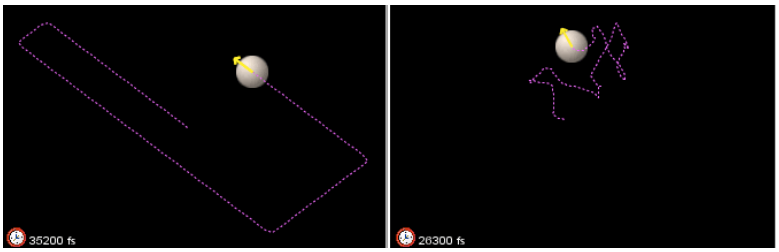


Three atoms. Students can see that chaos sets in when there are three atoms. It is possible to start with separated atoms and result in two being bound together, because once in a while, there is a complex interaction that results in the third atom carrying off a lot of kinetic energy In the example at right, it is possible to see that the potential energy has decreased as a result of the binding of the upper two, while the temperature increased and one flew off.





Brownian motion. The frames at right show two identical large atoms and the tracks they generate. The model on the right is filled with invisible atoms. This is the physical basis of Brownian motion.



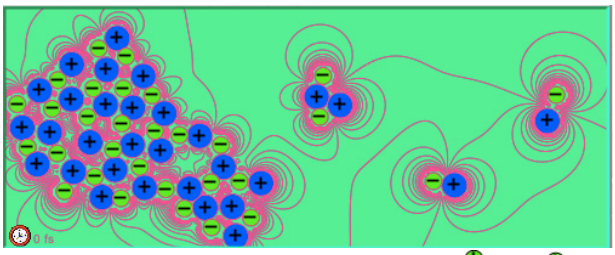
Buoyancy. It is possible to turn on a very strong gravity that simulates an ultra-centrifuge. A model that has two kinds of atoms or molecules, can result in separation on the basis of density.

Molecules

The Molecular Workbench supports much more than simple atoms. Atoms can be linked together to form molecules. The linkages simulate covalent bonds and are elastic, so they can store potential energy and vibrate. Atoms, either singly or in molecules, can carry charge, so it is possible to make ions, ionic bonds, and covalent bonds with dipole moments. As a rough approximation to larger molecules, big elliptical objects can be made, called Gay-Berne particles. These particles, unique to MW, have a kind of generalized van der Waals force and can be given an electrical dipole as well.

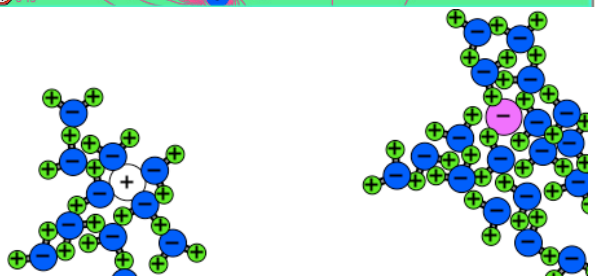
These additional functions greatly expand the range of physical phenomena that can be modeled, such as the following:

Non-crystalline solids. Texts normally teach that solids are crystals, but that is seldom the case. Most solids you see are amalgams, including wood, plastics, fabrics, our bodies, glass, ceramics, plaster, paint, and paper. Almost all large molecules condense into non-crystalline solids in MW.

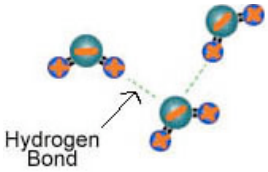


Ions and ionic bonds. Charging atoms can result in ionic crystals. The display at right shows the electric fields around ionic crystals. This system can be heated to get a plasma, the "fourth state of matter."

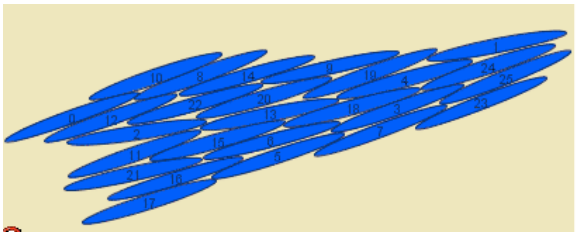
Ionic solutions. By placing ions into a model containing polar molecules, it is possible to model solvation. In the illustration at right, ions are surrounded by water molecules. The shell of water molecules surrounding each ion is like a solid than liquid and cannot dissolve another ion. It is apparent that ions can continue to dissolve in water until most of the water is tied up in these solid shells. This provides a model that explains the solubility of ions in polar liquids.



Hydrogen bonds. The MW model can show hydrogen bonds, if desired. Simply the mutual attraction of polar molecules, hydrogen bonds are particularly important in water because water molecules are so polar. Hydrogen bonds are critical in explaining the remarkable properties of water as well as crucial hydrophobic and hydrophilic properties of organic molecules.



Liquid crystals. Flat screen displays, calculator and digital watch displays, and most cell phones use liquid crystal displays (LCD). Liquid crystals form semi-crystalline structures that can be influenced by electric fields. All these effects can be modeled in MW using Gay-Berne particles.



Extensions to Chemistry

The models described to this point, while supporting chemical bonds, do not permit these bonds to be created or broken. MW also supports some chemical reactions. It would be too complex to support all possible reactions, so MW currently supports three specific kinds of reactions: a substitution reaction, a catalyzed substitution, and a polymerization reaction. These three illustrate most of the important properties of covalent reactions and homogeneous catalysts (Xie & Tinker, 2004).

Because molecular dynamics models are based on the physical interactions of atoms and molecules, it is necessary to model individual reaction steps rather than the overall reaction. For instance the generic reaction $A_2+B_2 \leftrightarrow 2AB$ is decomposed into the following five elementary steps:

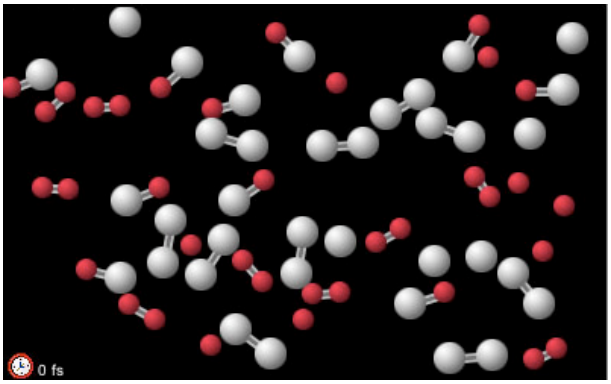
$$E_{AA} + A_2 \leftrightarrow 2A\bullet$$
$$E_{BB} + B_2 \leftrightarrow 2B\bullet$$
$$E_{AB} + AB \leftrightarrow A\bullet + B\bullet$$
$$A_2 + B\bullet \leftrightarrow A\bullet + AB$$
$$A\bullet + B_2 \leftrightarrow AB + B\bullet$$

where A• and B• are free radicals and the dots represent unpaired electrons. E_{AA}, E_{BB}, and E_{AB} are the energies required to pull the corresponding molecules apart, which are the energies released with the corresponding bond is made. In addition, there are activation energies associated with each of the last two reactions. The Molecular Workbench software allows the user to set all five of these energies. By changing the energies, the user can shift the equilibrium, determine reaction pathways, and alter the energy released.

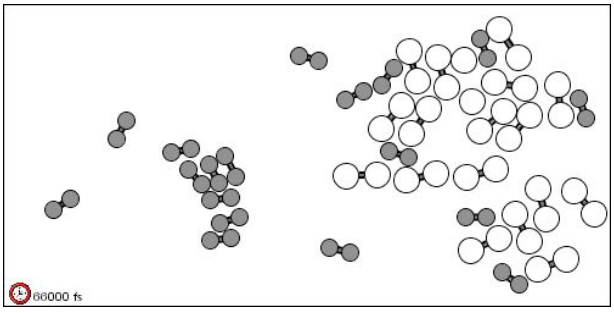
When a model is run, the program examines every existing bond to determine whether there is sufficient kinetic energy to overcome the energy barrier and break it, and every possible pair of atoms that are sufficiently close to see whether a bond can be made. The decisions are made on the basis energy conservation. As a result, models based on chemical reactions conserve overall energy, but can exchange thermal and chemical energy. This can provide a powerful explanation of enthalpy and free energy.

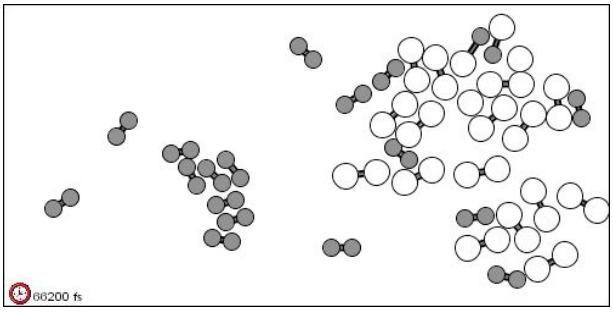
The following are examples of chemical models that can be created in the Molecular Workbench:

Equilibrium. When all the bond energies are equal and low activation energies, the system settles into equilibrium with about the same number of each molecule. But contrary to a common student misconception, the equilibrium is dynamic, with molecules being continually formed and broken. The student can change the energies and cause the equilibrium to shift. Students can also explore the effect of temperature on the equilibrium and the rate at which equilibrium is achieved.



Explosions. If the activation energies are high, the system can require a very long time to reach equilibrium unless the temperature is high. If the starting state much higher energy than the final state, it is possible to make an explosion. The frames below show an explosive mixture that had been slowly heated until the reaction began. The left screen captured in the upper right the very first disassociation of a molecule composed of two open atoms. The right frame shows the next instant in time when these two reacted with shaded atoms forming AB pairs and releasing considerable kinetic energy. This local heating rapidly

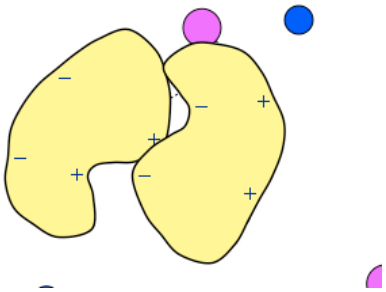


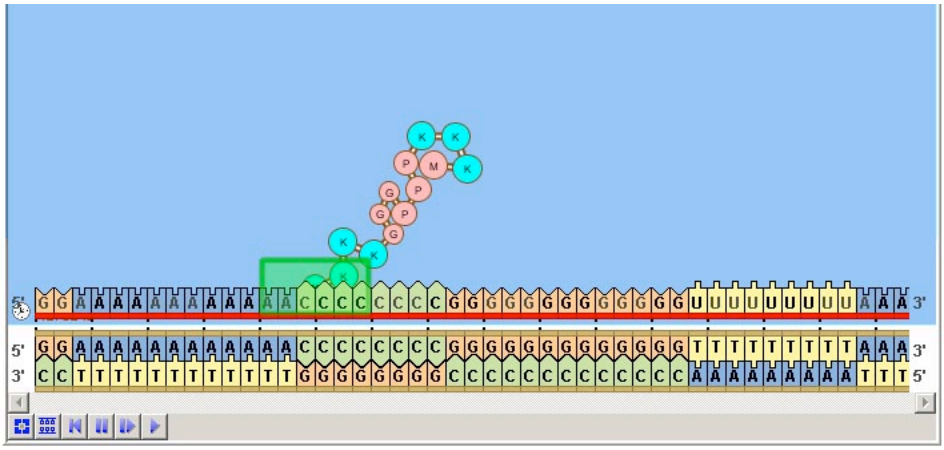


caused further disassociations quickly resulting in all the atoms forming AB molecules that were moving quite rapidly. This is a molecular description of an explosion. It also helps explain why some explosives can be stored safely.

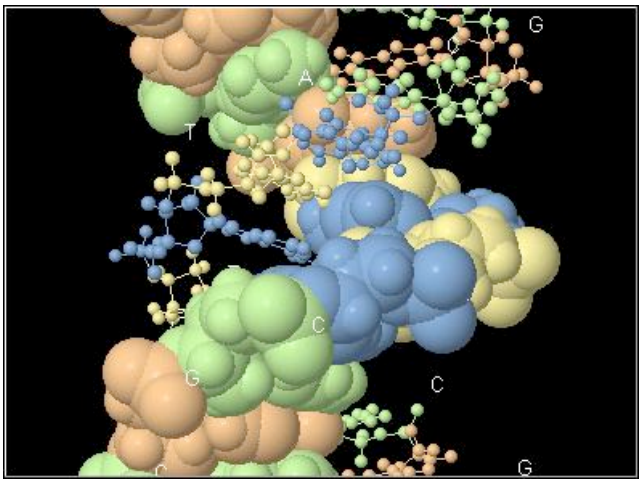
Extensions to Biology

We have made some important innovations in MW to extend molecular dynamics to biology. One involves "smart surfaces" that represent large bio-molecules. These can be drawn in any shape, filled or left as a ribbon, and "decorated" with charge. For example, at right, two similar bio-molecules are about to form a dimer, illustrating how complementary surfaces can match if their shapes and charge distributions are correct.





Another innovation is designed to support explorations of protein folding and the influence of solvents. Interactions of proteins with water would require excessive calculations because of the many water molecules required, so we introduce a pseudo force that approximates the effect of water or a non-polar solvent. The user can then put arbitrary polypeptide chains of any shape into these solutions and look at the resulting folding and the impact of temperature. The screen above is from an interactive model that supports these investigations. The "beads" that are growing from the moving translation area indicated by a green box, obey the physics of atoms, but represent individual amino acid bases for which charge and "hydrophobicity" can be set appropriately. This model reproduces the qualitative behavior of protein folding but cannot, of course, do it exactly, since that remains an unsolved problems problem.



This model also shows how DNA sequences code for proteins and how changes in DNA can change the structure of a protein. Students can edit a DNA fragment and see the effect on the protein coded by this fragment. Running the model shows how the DNA changes will result in different shaped proteins. Students can see that changes that result in amino acids with similar properties cause little change in the protein shape and hence, most likely, its function. However, other changes can make huge differences.

Another feature of our work that is important to biology have also incorporated a very flexible, free open source 3D molecular viewer called J-mol. [1] This is separate from MW and does not do molecular dynamics calculations, but can be built into MW learning activities. J-mol is very powerful, able to display and quickly rotate complex molecules in 3D. This capacity is illustrated above, where J-mol has been configured for different views of the two DNA strands. The ability of the user to rotate the structure by a mouse contributes to the perception of three dimensionality. While not part of MW, we use J-mol with MW models in our educational platforms.

[1] See http://jmol.sourceforge.net/

EDUCATIONAL CONSIDERATIONS

MW models can be used to illustrate all the phenomena described above and more, but if the software is used only to show students the models, then most of the educational value is lost. If the only goal of our research were to produce animations of atomic scale phenomena, a sophisticated model would not be needed..

For models to be of educational value, students must be able to interact with them. It is only through interaction that students can appreciate that the models, like reality, are based on a few general laws and that many different phenomena emerge from the application of these laws to different systems. This is a deep and important insight about science. In addition to its philosophical importance, the unity gained from such a perspective should help students understand a wide range of science topics and give the students the intellectual tools to predict new phenomena on the basis of the interactions of atoms and molecules. In our research we have seen evidence of this, where middle-grade students were able to explain diffusion after interacting with models of phase change (Pallant & Tinker, 2004).

Students could use the core Molecular Workbench software directly to explore models, but it is too complex with too many options for most students. Only dedicated or quite advanced students could make effective use of all its capacity. Our goal is to create self-contained learning activities with models that students can begin using right away, without having to learn more that absolutely necessary about the model. We also want these materials to be delivered online and coupled to student assessment systems. To realize these goals, we developed software that provides an educational platform for models in general and the Molecular Workbench in particular. MW has been linked to two different platforms: the MW Pages and Pedagogica (Horwitz & Burke, 2002; Horwitz & Tinker, 2001).

Both platforms provide the ability to create complete student learning activities that simplify the use of models, but also provide many other functions that educators need, including online delivery and student assessment. By providing these functions, we require that there is an activity author: someone who either creates or modifies the activities. The problem in creating authorware—software for authors—is to balance ease of use with functionality. Ideally, it would be easy for any teacher, textbook author, or curriculum developer to author or customize online activities that use MW. Customization is particularly important because it is always much easier to modify an existing activity that to create it from scratch. Customization is an excellent activity for teachers, because they know their students and curriculum and can make adjustments in an activity generated elsewhere to adapt the activity to the needs and strengths of their students. While undertaking this customization, teachers also can sharpen their understanding of the content of the activity, so it is an excellent form of professional development.

The two platforms available for MW differ primarily in their flexibility and ease of use. The MW Pages are easy to use and require no programming. Pedagogica is more powerful and permits more options, but requires programming in JavaScript. Student assessment with secure student registration is available only in Pedagogica. Each platform is under development and planned enhancements are drawing the two together. Pedagogica will soon support many functions without requiring JavaScript by using the word-processor approach developed by MW Pages. MW Pages will soon support student registration and secure assessment.

Molecular Workbench Pages

MW Pages is a browser-like environment that supports a special word processor. Because it mimics familiar browser and word processor applications, MW Pages is very easy for novice authors to use. Using pull-down menus and forms, models, model controllers, model outputs including a full-featured graphing tool, and other objects can be placed within text strings in the word processor. Model objects are located on the screen the way large characters would be, so it is easy to use spaces, tabs, and returns to position these. Other objects that are supported include J-mol html boxes, graphics, and hot links to other MW Pages. There is a full set of educational tools within the MW Pages environment that allow the student to take snapshots of the models and graphs, annotate the snapshots, and manage them. Other tools are available for creating and handling questions, uploading and sharing MW Pages, and creating and sending reports based on text, snapshots, and answers. For a full description of features see the MW Features Tour[2] and the user guide.[3]

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[2] See http://xeon.concord.org:8080/modeler1.3/screenshots/ss1.html.

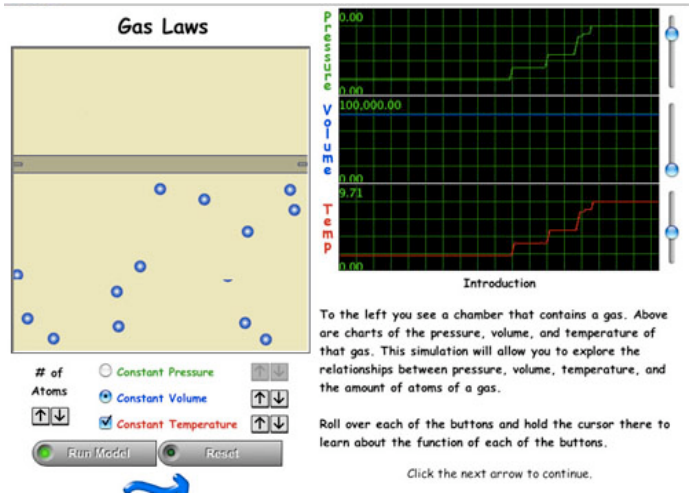
[3] The user guide is written in MW Pages. To launch the pages go to http://xeon.concord.org:8080/modeler/webstart/MW.jnlp and then once all the MW software installs itself, select "User's Guide." If you encounter difficulties go to the installation guide at http://workbench.concord.org/modeler/index.html.

The core MW container also has a number of options that are designed to simplify educational authoring. As illustrated below, the MW model can have an optional icon palette across the top of the model. The activity author can select which icons, if any, are displayed in the palette. In this way, the student is given just the controls that are useful for a particular activity and not others that might be irrelevant and confusing. Important functions can be introduced gradually in successive MW Pages until the student has fully mastered all the options. MW Pages also supports a macro language that allows an author to add considerable functionality.

Using these facilities, it is easy to author educational activities that use the MW model and to adapt these activities to different levels of students and different instructional objectives.

Pedagogica

Pedagogica is a platform initially developed for a genetics model—BioLogica—but is actually independent of any one model. The Molecular Workbench is one of many models that have been linked to Pedagogica. An activity in Pedagogica consists of one or more pages each with various objects. For instance, the illustration below shows a MW object on the left, a graphing object on the right, several button objects and some text objects. The author uses a graphical layout editor to place these objects on the screen. JavaScript commands determine the interactions between the objects and the appearance of each object type. Another tool helps structure the sequence of pages and the JavaScript that will be executed at each page and during the transitions between pages.



The activity illustrated had to be authored in Pedagogica because there is currently no way to measure pressure or to include a moving piston in the core MW application. These, and many other options were added to MW by running it under Pedagogica and programming the desired functions in JavaScript.

Because it is a full programming language, an author can do anything with Pedagogica. On the other hand, it does require programming in JavaScript and this severely restricts who can author.

Resources

Further information, models, and examples can be found at the Molecular Logic home page at http://molo.concord.org and in publications (Tinker, 2001, 2002, 2003; Tinker, Berenfeld, & Tinker, 2000; Tinker, Tinker, & Damelin, 2001). In the database link from this page there are over one hundred student activities that can be searched in a number of different ways. Most entries in the database provide descriptive information about the application, a screen shot, and a hot link to the actual activity. Some of these activities are single or linked MW Pages, while others are extensive Pedagogica-based lessons. The Molecular Logic page also has download information and links to all the software required. We encourage educators worldwide to create activities and submit them for publication on the database of activities[4] and to modify the models in that database to fit different educational needs.

CONCLUDING THOUGHTS

Our experience with the Molecular Workbench has demonstrated that computation models based on molecular dynamics can have wide application to science teaching across grades, disciplines, and topics. Molecular dynamics is

[4] See http://molo.concord.org/database/.

particularly adept at modeling phenomena that depend on thermodynamics in both equilibrium and non-equilibrium situations. The traditional approach of educators to equilibrium thermodynamics is to state as given the various equations that can be derived only when students master partial differential equations.

What we learned about educational modeling—

Of course, these impressions should be tested.

The Molecular Workbench represents an important kind of educational software with great potential.

Providing a large application such as MW with one or more platforms for the development and delivery of educational activities represents an important innovation. MW illustrates how powerful this can be for education. One application and two platforms has led to 200+ student learning activities

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