Authoring Molecular Dynamics Activities with Molecular Workbench

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Abstract: *Interactive molecular dynamics models, based on real time computation and visualization of behaviors emergent from molecular motion, are gaining ground in teaching physical science and molecular biology. Creating new models or editing existing ones, however, is difficult for educators whose primary focus is neither on computer programming nor on the computational science behind the scene. The authoring system of the Molecular Workbench software is specifically designed to meet this challenge. Built on top of a word processor, it can be used easily to build complex molecular dynamics models and author student activities in a way similar to creating a document using Microsoft Word.*

Keywords: educational software; interactive models; authoring; molecular dynamics simulation.

1. Introduction

Funded by the National Science Foundation, the Concord Consortium has developed a free educational molecular simulation program called the Molecular Workbench (MW) [1], which can be used to demonstrate many microscopic phenomena such as gas laws, phase transitions, chemical reactions, Maxwell speed distributions, Brownian motion, diffusion, osmosis, liquid crystals, crystallography, protein folding, molecular recognition, self-assembly, and much more.

The simulation engines of the MW software are primarily based on a computational technique called molecular dynamics (MD), which is a numerical method for solving the equations of motion for a system of atoms and molecules interacting with interatomic forces approximated from quantum mechanics of the system (Leach, 2001). The MD method was originally used only by scientists to understand atomic-scale phenomena, refine experimental data and engineer new products, and was introduced to education only recently[2]. While typical research-purpose tasks do not require the simulations to be manipulable, interactivity is important to education because it enables educators to design hands-on activities in which students can direct certain molecular processes (e.g. raising the temperature to melt a solid). The MW engines include substantial support for interactivity.

The strength of the MD models lies in their flexibility and extensibility, as they are based on fundamental principles of physics and chemistry. Models illustrating many different phenomena can be built or derived to simulate reasonably complex systems. Their applicability and educational potential is amplified with an authoring system that can be used to create models and student learning activities based on models. An easy-to-use authoring system will not only allow more educators to create novel models and modify preexisting ones, but also offer an opportunity to engage students in building models, which represents a shift of student interactions from the hands-on level to the heads-on level.

We have built an authoring system that is seamlessly integrated into MW. This paper will introduce this authoring system, present the architecture, and discuss its applications to science education.

2. The Convolution of Molecular Dynamics Models with a Word Processor

The importance of models in education is widely accepted in education and is explained by the abundance of interactive multimedia on the Internet. It is usually difficult to modify a model, however, because programming skill is often needed to change the code. Many teachers are interested in modifying the pedagogy that involves using models, and would like simply to be able to contextualize the models and adapt them into their own curricula. This may be as trivial a change in an activity as rephrasing a sentence, adding a paragraph that speaks to a specific group of students, inserting assessment questions, making connections to in-class activities, changing the color or the layout to enhance attentions, or simply translating into their own languages.

What is needed for these common purposes is a simple tool for editing pedagogy that supports models in context. To achieve this goal, we have invented an architecture based on the convolution[3] of the modeling engines with a word processor (WP). In this architecture, a model is represented in the data structure by a character with a set of attributes that specifies the model. It is handled as if it was a regular character by the WP, but is actually rendered in its own graphical form and remains interactive through its own user interface. If we view such a file as a mathematical function of the position of character, it is precisely the effect of convolution of one set of structured data (text) with another (embedded models). Thus, this architecture permits models to be wrapped by text and inserted into or deleted from text in exactly the same way a character gets added or removed in a WP, meanwhile still allows the models to be operated as if they were standing alone. This makes it easy to create interactive models with surrounding instructions, which we call activities.

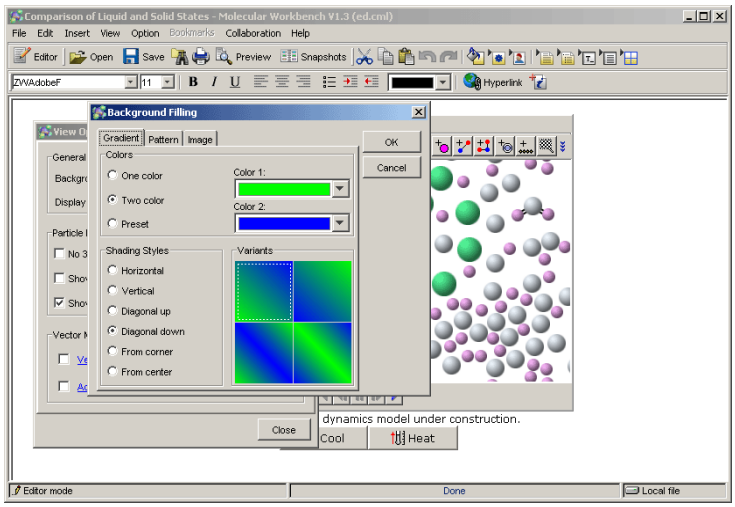

Figure 1. The user interface of the MW authoring system is similar to that of a WP. Here is a screenshot that shows a user interface for changing the background of a model. It also shows the usual tool bar buttons for operating and editing documents.

By default, a model will be empty when inserted in to a page. As soon as displayed on the page, it can be edited using its own user interface, which provides dozens of actions that can be used to create atoms, construct molecules, define properties, manipulate objects, input/output content, and so on. Similar to the buttons in the tool bars of Word, each action in MW can be hidden or shown. When an action is needed, it can be pulled from a list, and then be delegated by a button in a tool bar attached to the model. The actions can be removed after the model is constructed, or kept in the tool bar for use by the activity users.

An author has available both a wide variety of controllers for the user to interact with the models and outputs of the MD engines for the user to analyze the simulations. Controllers and outputs can also be convolved into the WP. Controllers, such as temperature, energy parameters or external fields, are connected to the model, enabling

the author to design easy ways to interact with the model. Outputs can also be placed on a page to show the results of a simulation. For example, concentrations of reactants and products can be shown in a graph to visualize the reaction rates of a chemical reaction. Being able to author controllers and outputs is a useful feature resulting from the "convolution" architecture. Teachers often have difficulty in implementing a curriculum that involves using a tool with a complex user interface, because students can be overwhelmed by the hierarchical menus and the many buttons and popup windows, and as a result, waste their time wandering through something irrelevant to the subjects they are supposed to learn. For both teachers and activity designers, the instructions for getting to the controls or outputs that are placed in menus and dialog boxes may become unnecessarily complicated, making the curriculum hard to implement. With the MW authoring system, an activity designer can show only the controllers and the outputs needed for the activity. Hence, the user interface becomes more succinct and friendlier, and the instructions for operating the models are simplified.

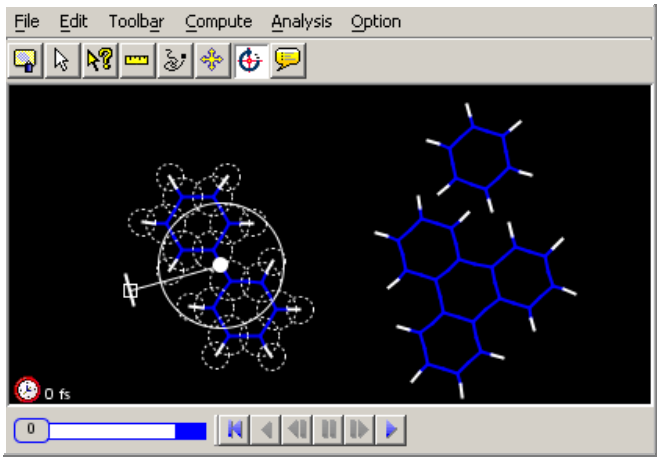

Figure 2. A screenshot of a model that has a tool bar and a menu bar. The model is in a state that allows the user to rotate a molecule. The page in which it is embedded is not shown.

3. The Viewing Mode and a Library of Demo Models

The MW software has two modes: the viewing mode and the authoring mode. The authoring system is disabled in the viewing mode, which protects the content from changes. In the viewing mode, MW is a special browser that delivers models and activities in exactly the same way a conventional web browser delivers content. In the main page of this browser, we have deployed many demo models that educators can adapt and use in their own activities. These demos are categorized, and can be used as a library of models, growing as more models are developed and added. The library covers many science concepts across all subjects, including classical mechanics, intermolecular forces, states of matter, materials science, water and solution, chemical reactions (Xie and Tinker, 2005), proteins and DNA (Berenfeld et. al., 2004), and so on. If a model in this library is saved to a disk, it becomes modifiable, allowing the authoring mode to be invoked. Students can derive their own variations from it. Teachers can create activities based on it to use in their classrooms.

4. Collaborative Learning and Assessment

Once the user creates a model or an activity, it can be uploaded to a web folder to be shared with other people. More easily, it can be uploaded to our database directly using the collaboration facilities available on the MW user interface. All the uploaded models and activities can be viewed by anyone using MW. This creates an opportunity

for users to share their creations. It has many other potential applications as well. For example, it would be worthwhile to engage students in building models in a collaborative setting where models can be shared, commented and revised, and investigate learning through co-designing models. Students can also be asked to build models independently to solve a set of problems. On the research side, studying students' uploaded models may provide rich information about their reasoning progresses with models. These investigations would not have been feasible without an authoring system.

The authoring system also allows MW to serve as a tool for assessment. Student thinking can be captured using traditional short answers and multiple-choice questions, which can be put into an activity using the authoring system. A database of annotated snapshot images students take of the models and put into a file with text describing their observations using the authoring system while going through an activity can be used to probe student learning. Furthermore, a database of models designed by students could provide insights into how they reason with models and how well they grasp the variables involved.

5. Concluding Remarks

Students from all over the world have used the MW software, and have uploaded thousands of reports to our database. In the field tests recently carried out by researchers at the Concord Consortium, it has been found that the use of MW materials can significantly improve student understanding about molecular concepts (Pallant and Tinker, 2004). With the powerful authoring system presented in this paper, we expect more users will use it to create new molecular models and promote the molecular literacy --- the knowledge of the atomic-scale world, as this kind of knowledge is increasingly important in the eve of the nanotechnology revolution.

Finally, it has to be pointed out that the "convolution" architecture of the authoring system can be applied to any kind of models besides the MD models it was originally designed for. In fact, our long-term goal is to develop it into a versatile modeling and simulation platform capable of supporting a considerable part of science education based on a set of fundamental principles of science.

Footnotes

[1]The Molecular Workbench software web site: http://workbench.concord.org/modeler/index.html

[2]In the late 90s, the National Science Foundation funded two independent groups, one at Boston University and the other at the Concord Consortium, on exploring the application of MD models to education. There is also a commercial MD product available (http://www.starkdesign.com).

[3]Convolution, meaning the blending of two functions, is a term borrowed from mathematics.

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