

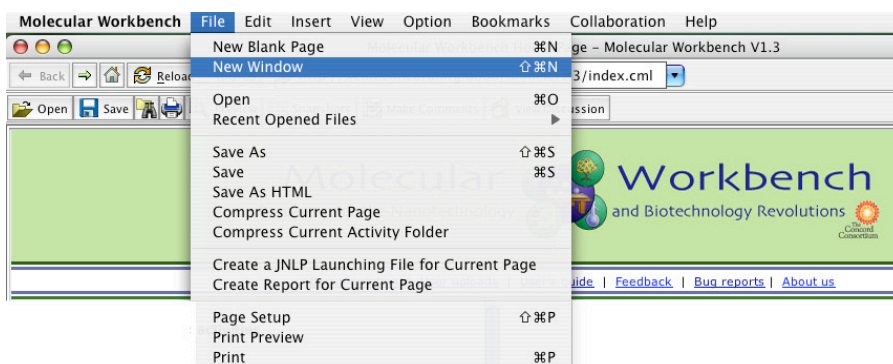
QUICK START GUIDE - Illustrated: Making a Model

How to use the Molecular Workbench to build a model from scratch

1. Open a New Window.

First, open a new MW window by selecting:

File->New Window



2. Make a blank page and save it.

In the new window, select:

File->New Blank Page

Let's go ahead and save it now. Make a new folder for your model and save it there. Remember to save occasionally as you work. Of course, you can use **Edit->Undo** to go back a step if you make a mistake!

3. Title the page.

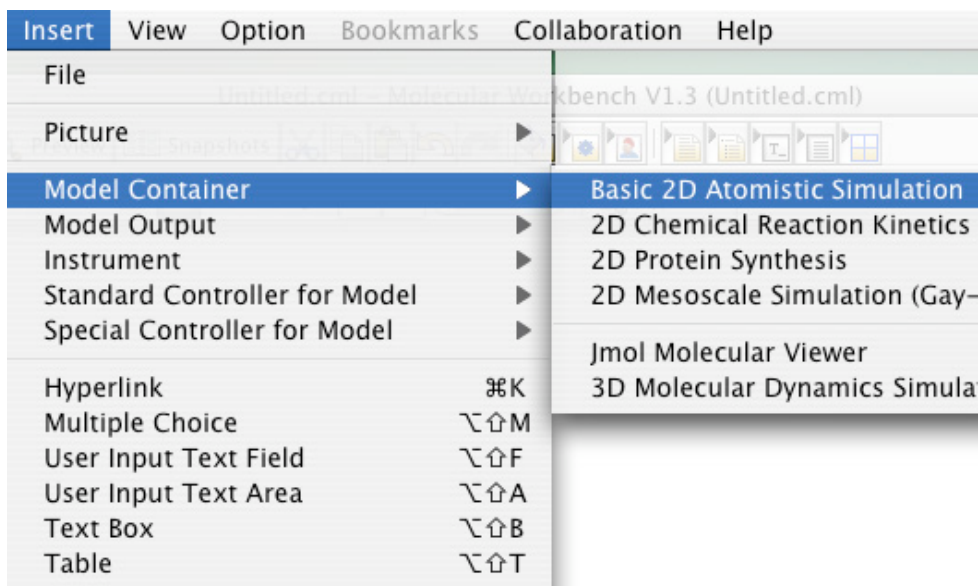
You can write text right onto the page and set its font, font size and color. Try adding some text now, perhaps a title and an introductory paragraph.

4. Insert a model container

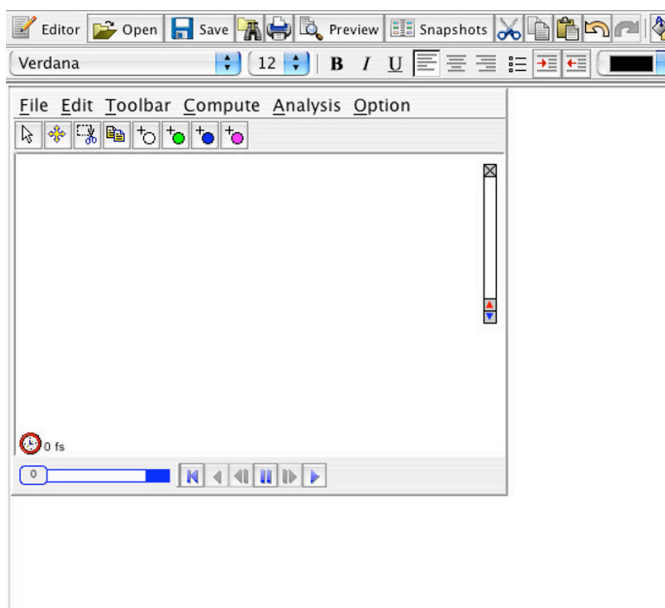
The next step is to drop a container for a model onto the page. Controls for pages are at the top of the Molecular Workbench. Go to INSERT in the top menu, between EDIT and VIEW. There you will find many objects to insert. The easiest one to start with is the Basic 2D Atomistic Simulation.

Go to:

Insert->Model Container->Basic 2D Atomistic Simulation



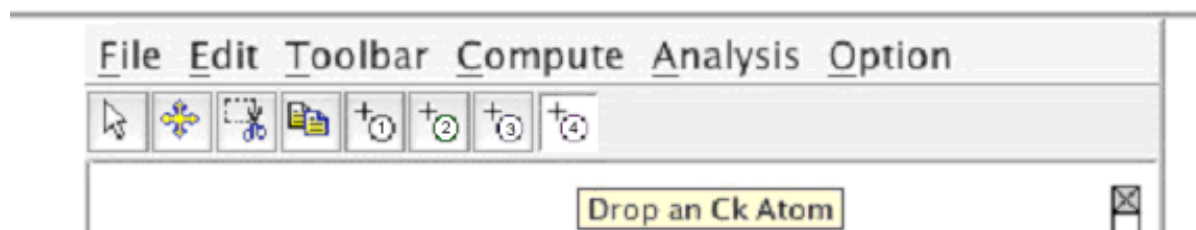
You will get:

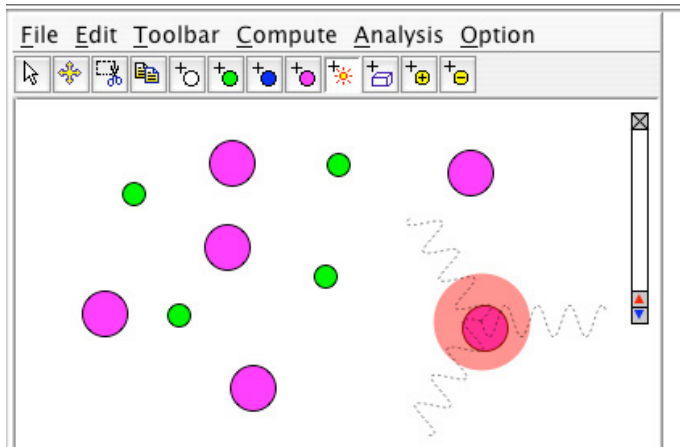


The container comes with its own menus and some controls already in its toolbar.

5. Customize the container's toolbar

Each model has its own menu bar, and below that, a row of buttons called the toolbar. Hover your mouse over any button to get a "tooltip."





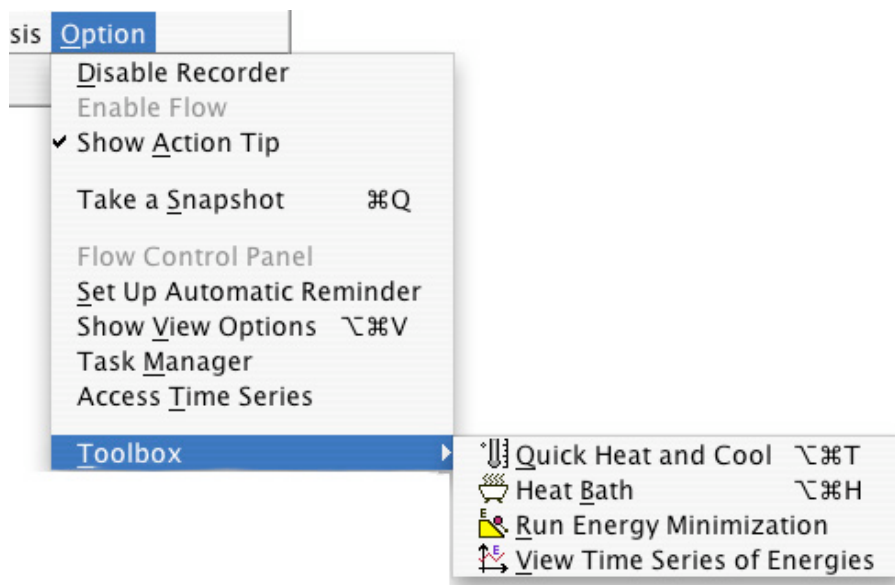
8. Controlling Temperature

Heat bath A very useful tool for stabilizing your model is called the "heat bath." It forces the whole model to stay at a fixed temperature. When your model is behaving strangely, it sometimes helps to turn on the heat bath.

From the model container's menu bar go to:

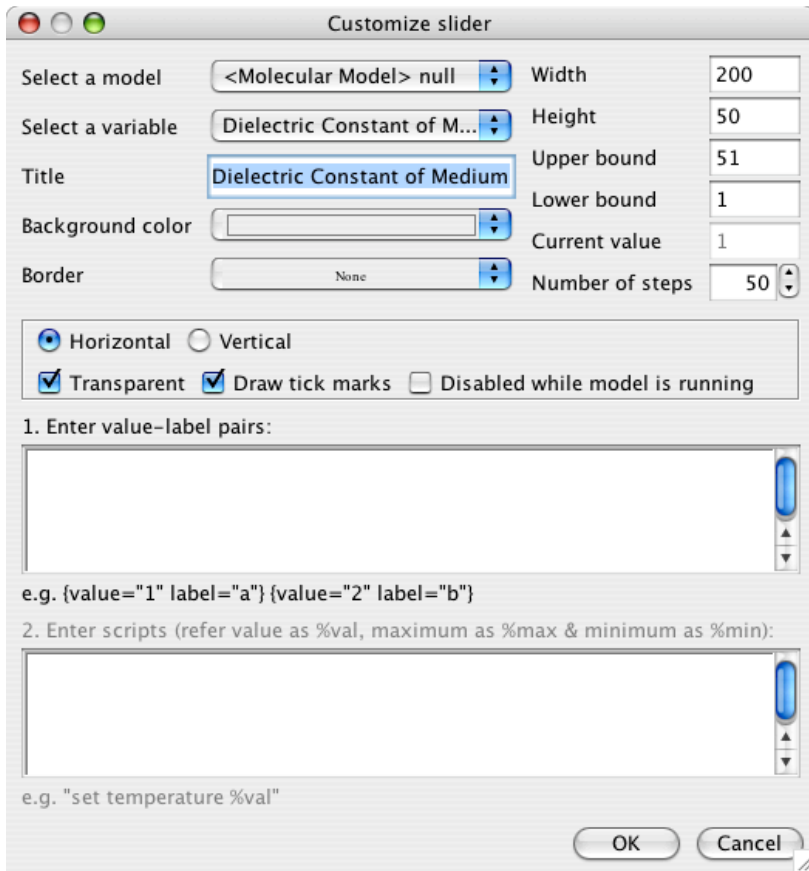
Option->Toolbox->Heat Bath

Then, check "apply" to turn it on, and set a temperature (in degrees Kelvin; 1000 works well).



Temperature Slider. You can adjust this temperature while the model runs by adding a slider component to the page.

On the page menu bar go to: **Insert->Standard Controller for Model->Slider**



Next to "Select a Variable", pick "Temperature", near the bottom of the list.

This creates a slider at the position of the cursor. You can move it around, by hitting enter, or by selecting it and pressing the button that centers text. You can also modify it by right clicking (Windows) or Apple-clicking (Mac) on it.

Other controllers. Notice that in the "Standard controller for a model" menu there are several other model controllers, such as on/off buttons, check boxes and radio buttons, which can control many model parameters.

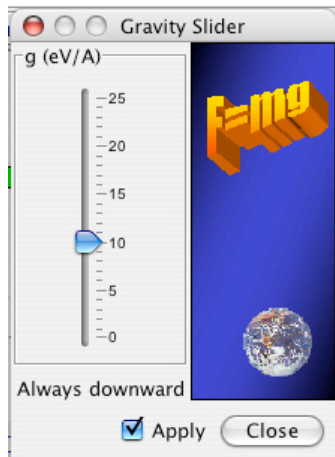
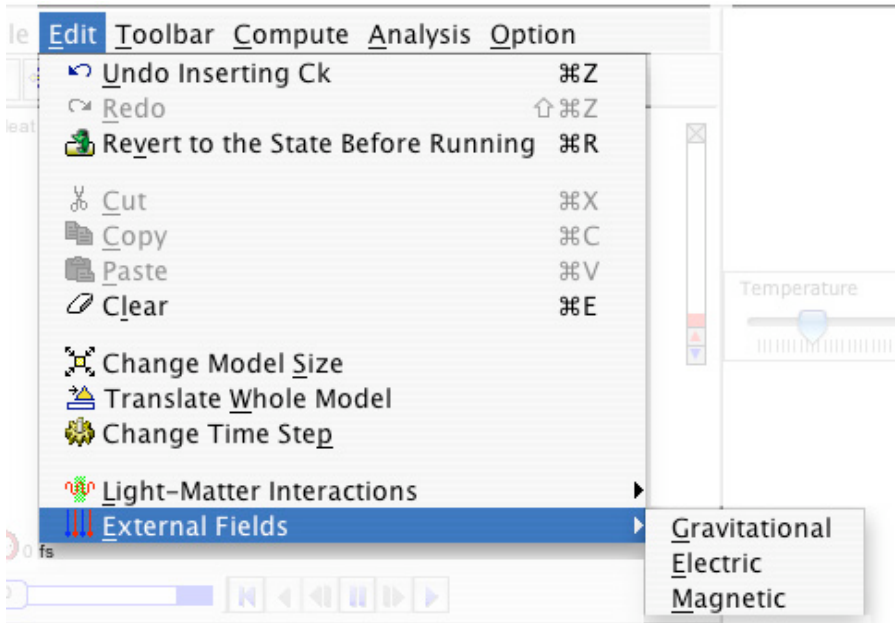
9. Turn on gravity

Now, we'll make our atoms fall down.

From the model container's menu bar go to:

Edit->External Fields->Gravitational

Check "apply" to turn it on, and then set the strength of gravity you'd like.



You can also create a **check-box** on the page for turning gravity on and off. On the page menu bar go to: Insert->Standard Controller for Model->Check Box
 Next to "Select an Action" pick "Gravitational Field."

Gravitational Field


Congratulations! You have begun to model!

10. Try Making Other Types of Models




Now you can start making your own models. It may be helpful to select from the model container's menu: **Toolbar->Add All Available**, so you can quickly access all the tools at once.

Here are some ideas to get you started:





Brownian motion

Add lots of blue atoms⁺, and one purple one⁺. Watch the purple one's erratic path. Show its path using the "trajectory" tool ( in "non-editing actions").


Ionic crystallization

Add one purple $^{+}$ and one blue atom $^{+}$. Use the charge tools ( and ) to make one +1 and the other -1. Use the duplicate tool  to make many copies of each.

Water

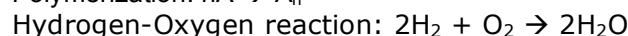
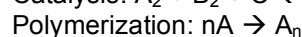
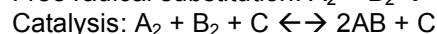
Use the "drop a triatomic molecule" tool , then charge your molecule ( and ) so it's water-like and duplicate  it many times.

Phase change

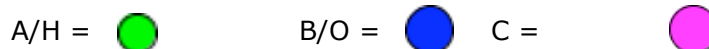
Drop in a bunch of atoms using the "fill" tools (e.g. ) and experiment with temperature. Do you see liquid, solid and gas phases?

Chemical Reactions

Insert a chemical reactions model by going to, on the page menu bar, Insert->Model Container->2D Chemical Reaction Simulator. Explore the model's Reaction menu. There are several kinds of reactions which can be modeled:





For all of the above reactions the atoms the default atoms are:





You can add controllers to allow easy user adjustment of dissociation energies and/or activation energies by using the Insert->Special Controller for Model -> Chemical Reaction Kinetics menu.

Protein Folding

Try out the "add an amino acid" tool . Build a chain of amino acids by click in one place several times. Switch to the "select object" tool , and alt-click an amino acid to change types. From the page menu bar select *Insert->Standard controller for model* to add combo boxes for "show properties" and "solvent type."]

DNA

Try the "add a nucleotide" tool . Build a DNA strand by clicking in one place several times. Switch to the "select object" tool , and alt-click a nucleotide to change types. Make two complementary strands.

Protein Synthesis

Insert a protein synthesis model by going to, on the page menu bar, Insert->Model Container->2D Protein Synthesis Simulator. At the bottom of the model, the second button lets you enter a DNA sequence. Press run to watch transcription and translation!

Tips on customizing for student use

Once you've made a model, you can build an activity around it. Here are some simple things that we've found help in adapting models for activities. They basically involve limiting the number of options the students see, so they can focus on the activity:

Customize or remove the toolbar

You may want students to interact with your model using some of the tools, e.g. having them add their own atoms. Give them only the tools they need.

Disable the recorder

The recorder is a feature that stores time series data for the model, so you can go back and watch it again, and also for use in various analyses. Many activities don't need this, so you can shut it off (and simplify the interface as well) by going to:

Option->Disable recorder

Hide the menu bar

Hide the model's menu bar by right clicking (windows) or apple-clicking (mac) on it (away from the menus), and selecting "show menu bar" so that it becomes unchecked.