



Scientific Computing & Modelling

ReaxFF Tutorial

**ADF Program System
Release 2010**

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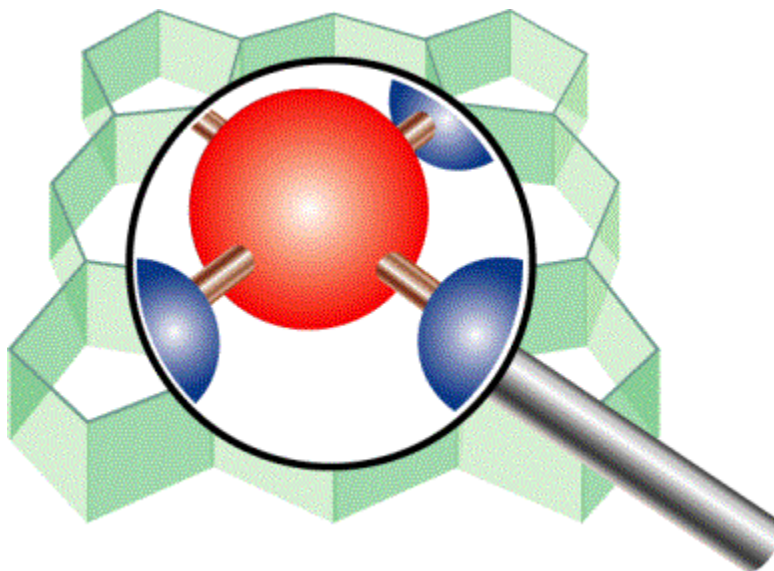


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Introduction

This document will provide a hands-on tutorials demonstrating ReaxFF. We do this using a graphical user interface (GUI). Parts of the GUI are intended for ReaxFF only, for example ReaxFFinput. Other parts (like ADFmovie) are also used for other software in the ADF package. The purpose of the tutorials is to give a quick tour of how to use ReaxFF via the GUI.

The first tutorial provides you with an overview over all relevant GUI modules. It will also show you some basic editing of your input structures, and the reactive feature of ReaxFF.

The editing features of ReaxFFinput are identical to those of the ADF-GUI. If you are not familiar with the ADF-GUI, we suggest strongly you try some of the [ADF-GUI tutorials](#) (especially numbers 1 and 4).

The second tutorial will show you how to set up a more complex system and how to use some of the advanced features of ReaxFF. In setting up the system you will also use BANDinput to create an aluminum surface.

Additional information may be found in the [ReaxFF Reference manual](#)

ReaxFF GUI modules

The ReaxFF GUI is the Graphical User Interface for ReaxFF. It consists of ReaxFFinput and several modules also used for the ADF-GUI and BAND-GUI:

ADFjobs

This utility (`$ADFBIN/adfjobs`) manages your jobs: run a job on your local machine or on remote machines. It also serves as an interface to all files belonging to your job, and it serves as a convenient launcher of the other GUI modules.

ReaxFFinput

ReaxFFinput (`$ADFBIN/reaxffinput`) helps ReaxFF users to easily create ReaxFF jobs. You can use ReaxFFinput to define your molecule (geometry), and to set details of your ReaxFF job using an easy-to-use graphical user interface. ReaxFFinput will generate the basic job script for you. This script takes care of running ReaxFF as required.

ADFmovie

ADFmovie (`$ADFBIN/adfmovie`) follows geometry steps (thus, trajectories) as generated by all programs in the ADF package, including ReaxFF. In addition, it can show graphs of most of the properties that ReaxFF calculates. It can be used to monitor the progress of a simulation (while the simulation is still running), or it can be used to analyze the results after your job has finished.

ADFTail

ADFTail (`$ADFBIN/adftail`) shows the contents of a text file, updating when the text file grows (like the UNIX `tail -f` command). It is used to monitor the 'logfile'. The progress of a ReaxFF calculation is always written to this file.

GUIprefs

GUIprefs (`$ADFBIN/guiprefs`) allows you to adjust and save numerous GUI preferences, such as color schemes, environmental variables, etc. All GUI modules will use these preferences.

BANDinput

BANDinput (\$ADFBIN/bandinput) allows you to set up a BAND calculation. It also contains tools to build crystals and slabs (surfaces). For this reason it is often useful together with ReaxFFinput.

All GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using the SCM menu commands you can easily switch between the different modules needed for ReaxFF.

Starting the ADF-GUI modules

We will assume that you have installed the ADF package on your machines.

Depending on your platform, you start the ADF-GUI modules in a slightly different way:

UNIX (such as Linux) users

In this tutorial we will assume that you have added \$ADFBIN to your PATH. We advise you to do this if you have not already done so. If you do not wish to add \$ADFBIN to your PATH, you must start the utilities using

```
$ADFBIN/adfjobs &
```

instead of just

```
adfjobs &
```

On all UNIX platforms, including Mac OS X, the ADF-GUI programs are XWindow (X11) programs. Your environment should have been set up correctly to run such programs. In particular, you need to make sure that your DISPLAY environment variable has been set properly.

You can test this easily by starting a simple X program from your shell:

```
xcalc &
```

Assuming the xcalc program is in your \$PATH, a small window should appear with the image of a calculator. If not, please consult your local system administrator for additional help. Typical problems have to do with your DISPLAY variable, and with security issues when trying to connect to the X server.

Windows users

In this tutorial we will assume that you have installed the ADF package using the Installer with all the options set to default.

You can start the ADF-GUI (adfjobs) by double-clicking its icon on the desktop.

Macintosh users

Macintosh users have several easy ways of starting the ADF-GUI modules: just like on any other UNIX system (thus, using the command line), or using the ADFLaunch program.

The easiest way is using the 'ADFLaunch' program. When you start it, ADFjobs will be started automatically. Next you can use the SCM menu to start the other ADF-GUI modules.

Tutorial 1: Burning methane and ethanol

This tutorial will help you to:

- create a simple molecule (ethanol)
- create a simple mixture (methane and oxygen)
- set up to burn it quickly (set up your ReaxFF simulation)
- burn it: perform the actual ReaxFF simulation
- visualize what is happening during and after the simulation

Step 1: Preparations

Start ADFjobs

On a Unix-like system, enter the following command:

```
cd
adfjobs &
```

On Windows, one can start ADFjobs by double-clicking on the ADF-GUI icon on the Desktop:

Double click the ADF-GUI icon on the Desktop

On Macintosh, use the ADFLaunch program to start ADFjobs:

Double click on the ADFLaunch icon

Make a directory for the tutorial

We prefer to run the tutorial in a new, clean, directory. That way we will not interfere with other projects. ADFjobs not only manages your jobs, but also has some file management options. In this case we use ADFjobs to make the new directory:

Select the **File** → **New Directory** command (thus, the New Directory command from the File menu)

Rename the new directory by typing 'Tutorial' and a Return

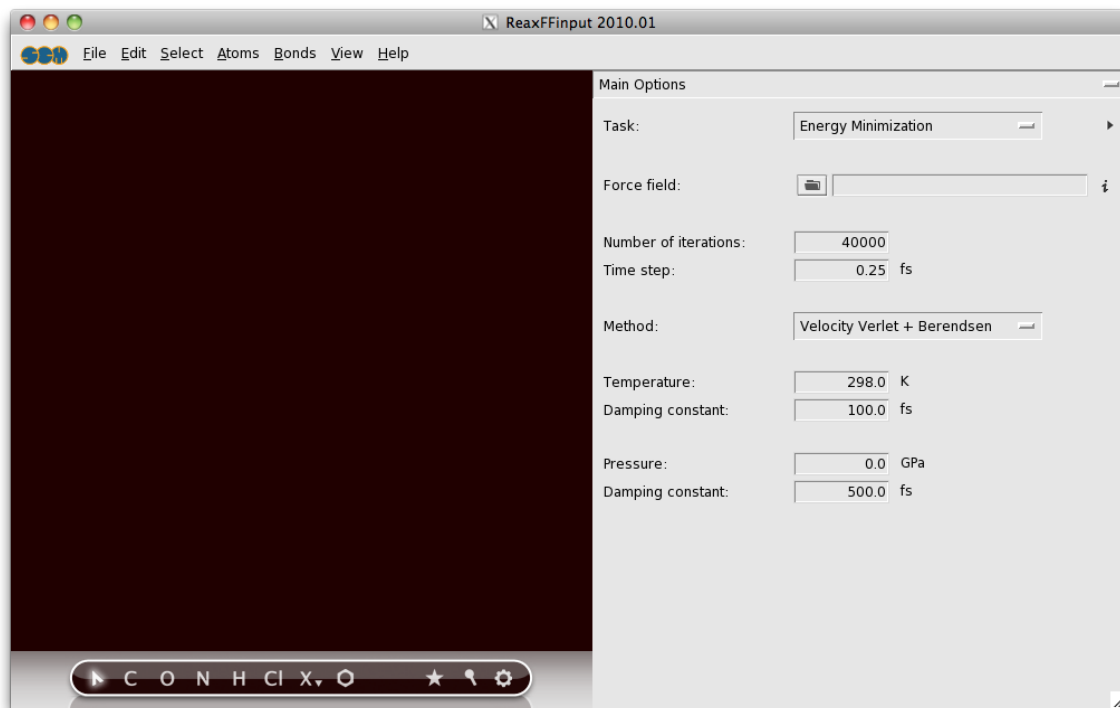
Change into that directory by clicking once on the folder icon in front of it

Start ReaxFFinput

Now we will start ReaxFFinput in this directory using the SCM menu:

Use the **SCM** → **ReaxFF input** menu command

The ReaxFFinput module should start:



The ReaxFFinput window consists of the following main parts:

- the menu bar with the menu commands
- the drawing area of the molecule editor (the dark area on the middle left side)
- the status field (lower part of the dark area, blank when the ReaxFFinput is empty as shown above)
- the molecule editor tools
- many panels with several kinds of options (currently the 'Main Options' panel is visible)

Undo

ReaxFFinput has an Undo command, which works on your molecule (thus not on your input options).

<u>U</u> ndo	Cmd Z
<u>R</u> edo	Shift Cmd Z
<u>C</u> ut	Cmd X
<u>C</u> opy	Cmd C
<u>P</u> aste	Cmd V
<u>C</u> lear	Cmd B
Remove Molecules Outside Cell	
Map Atoms Into Cell	
Set Cell Center	
Generate Super Cell...	
Set Origin	
Symmetry	▶
Mirror	▶
Align	▶

If you make a mistake while making changes to your molecule, just use the **Edit** → **Undo** menu command to go back in time. You can Undo more than one step, or Redo a step (with **Edit** → **Redo**) if you wish to do so.

Step 2: Create ethanol

To show you how to create new molecules, we will start by making a single ethanol molecule.

The molecule editor is identical to the molecule editor in ADFinput.

For a long and detailed tutorial on the builder, please check the [ADF-GUI tutorials](#).

Click on the C-tool

Click once in the drawing area: a carbon atom should be drawn

Click a second time in the drawing area, next to the carbon atom just created:
a second carbon atom connected to the first one

Click on the O-tool

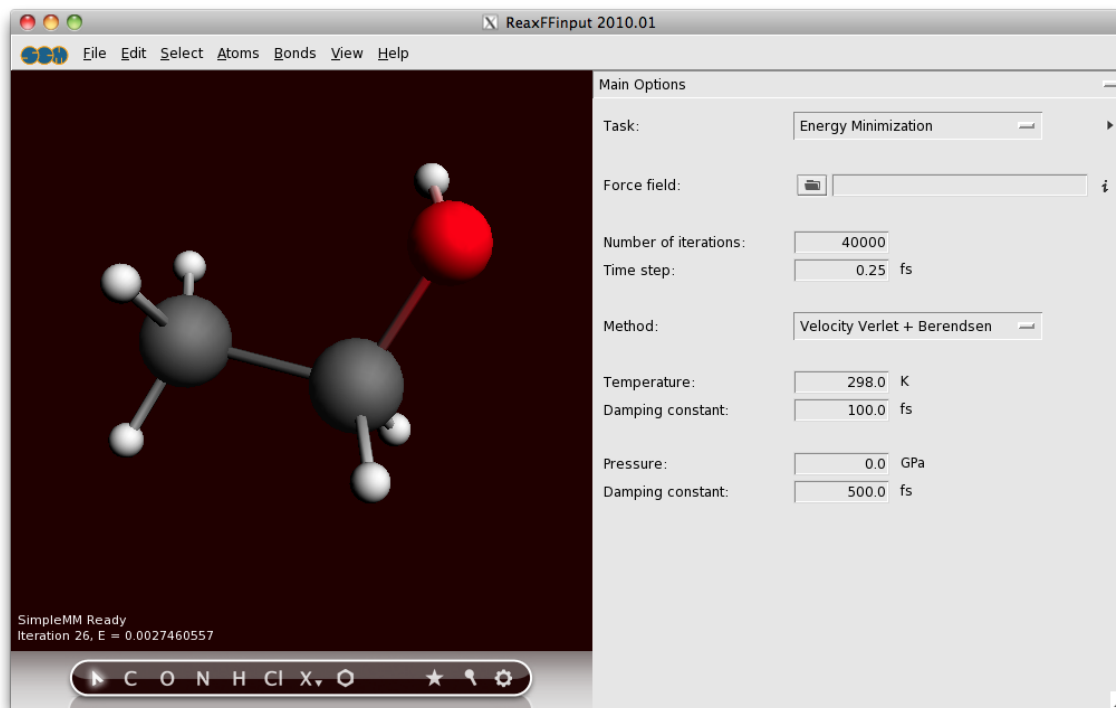
Click in the drawing area, next to the second carbon atom: an oxygen atom will be added

Press ESC to go back to the pointer tool

Click in empty space to clear the selection

Use the **Atoms** → **Add Hydrogen** menu command to add hydrogen

Click the optimize button (the gear-like button on the bottom)



You now should have a single ethanol molecule.

You can move your molecule using the mouse, again identical to the ADF-GUI modules:

Click once somewhere in empty space to make sure nothing is selected.

Click with the left mouse button, and drag:
your molecule will rotate.

Click with the left mouse button with the ctrl-key, and drag:
your molecule will rotate in-plane.

Click with the middle mouse button (or left with alt-key), and drag:
your molecule will be translated.

Click with the right mouse button (or left with command key), and drag up and down:
you will zoom closer to or away from your molecule.

Use the scroll-wheel on your mouse, if you have one:
you will zoom closer to or away from your molecule.

Step 3: Add your Methane / Oxygen mixture

Next we will add methane and oxygen to your molecule. For full combustion we need at least 2 oxygen molecules for each methane molecule. So we will add (to your ethanol molecule) 100 methane molecules and 250 oxygen molecules.

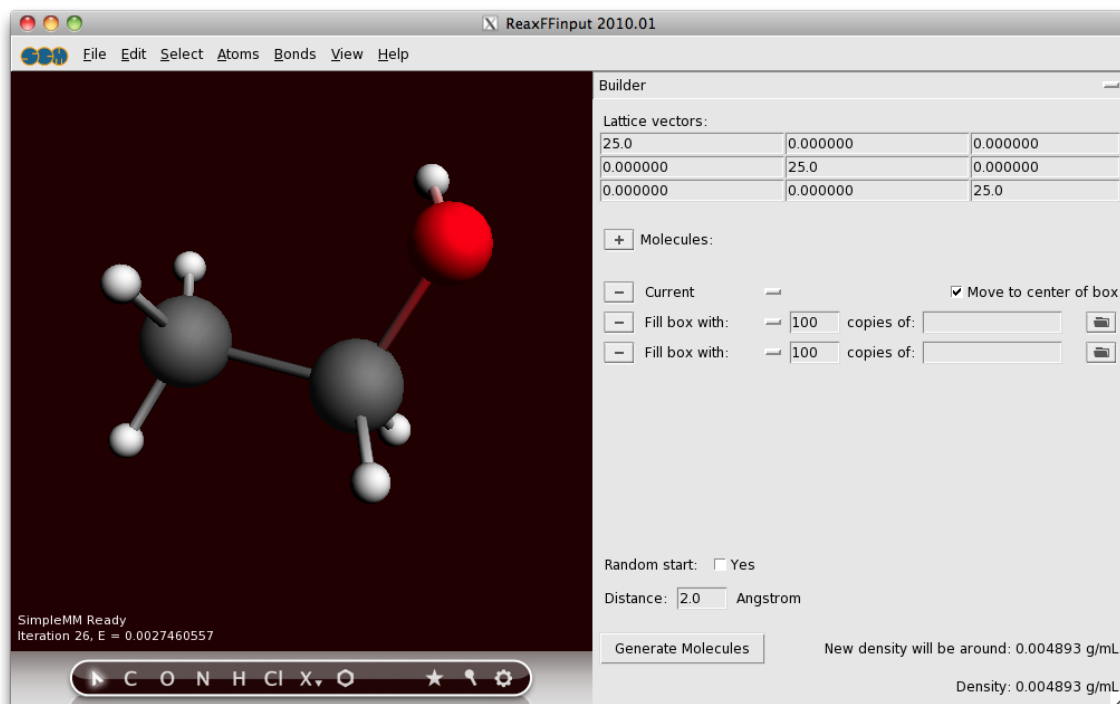
On the right hand side, use the pull-down menu on the top (currently reading 'Main Options') to select the 'Builder' panel

The Builder allows you to build your system, and set some things like the cell vectors that define the computation cell. ReaxFF always uses periodic boundary conditions. The default cell is a cube with sides of 25 Angstrom.

Next you can use the Builder to add many molecules, randomly distributed. In the list of molecules to be added the Current molecule is already present. This will make sure that your ethanol molecule will be part of the final system. However, we want to move it to the center of the simulation cell:

Check the 'Move to center of box' check box on the 'Current' molecule line in the builder

Click the + button in front of 'Molecules' twice to add extra molecules (once for methane, and once for oxygen)



Click the file select button on the first 'Fill box with' line (it looks like a folder)

Select Methane.xyz

Click the file select button on the other 'Fill box with' line

Select O2.xyz

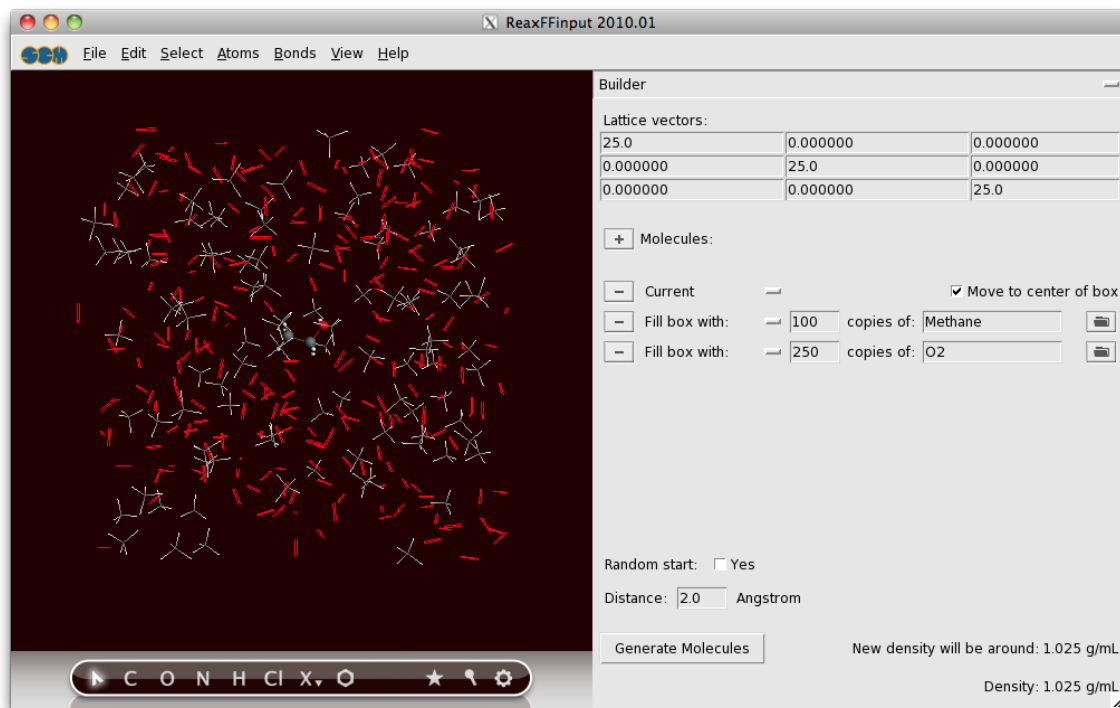
Change the 100 in front of the O2 to 250

You now have specified how the builder should build your system: the ethanol molecule, with methane (100 times) and oxygen (250 times) added.

At the bottom of the Builder panel you can see that the current density is very low (only an ethanol molecule in your cell). The new density, after adding methane and oxygen, will be around 1 g/mL, which is obviously very high for this mixture. For this tutorial that is fine as it means things will happen faster.

Next we will actually generate the molecules:

Click the 'Generate Molecules' button



The molecules are generated at random positions and orientations, with constraint that all atoms (between different molecules) are at least the specified distance (2.0 Angstrom) apart.

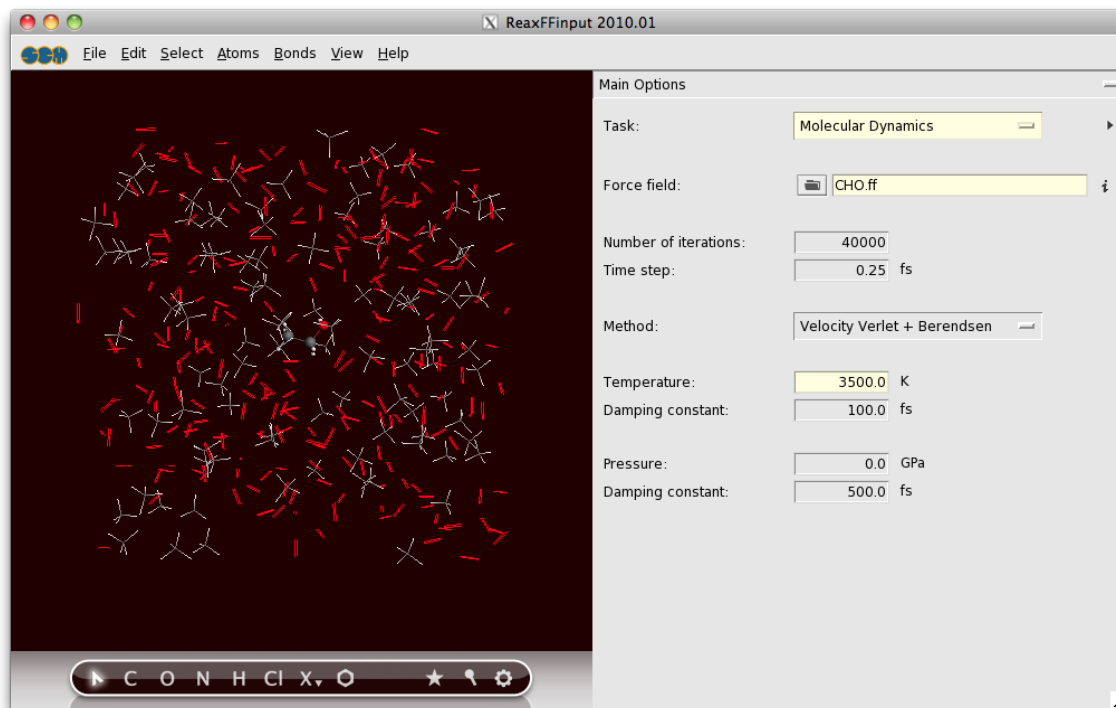
Step 3: Prepare for burning: set up the simulation

The next step is to set up the details of the simulation. For this tutorial we will perform an MD simulation, at very high temperature and density. This is to make things happen quickly. Obviously it is not a realistic system.

Select the 'Main Options' panel
 Choose the 'Molecular Dynamics' option from the Task pull-down menu
 Specify a temperature of 3500 K
 Click the 'i' on the right side of the Force field line

A new window should appear describing what force fields are available, including a short description and references. For this particular example we will use the CHO force field for hydrocarbon oxidation.

Close the window describing the force fields
 Click on the folder-like button in the Force field line
 Select the CHO.ff force field file



Step 4: Burn it: run the simulation

Now we will run your set-up:

Use the **File** → **Run** command

When asked to save your input, save it with the name 'Methane'

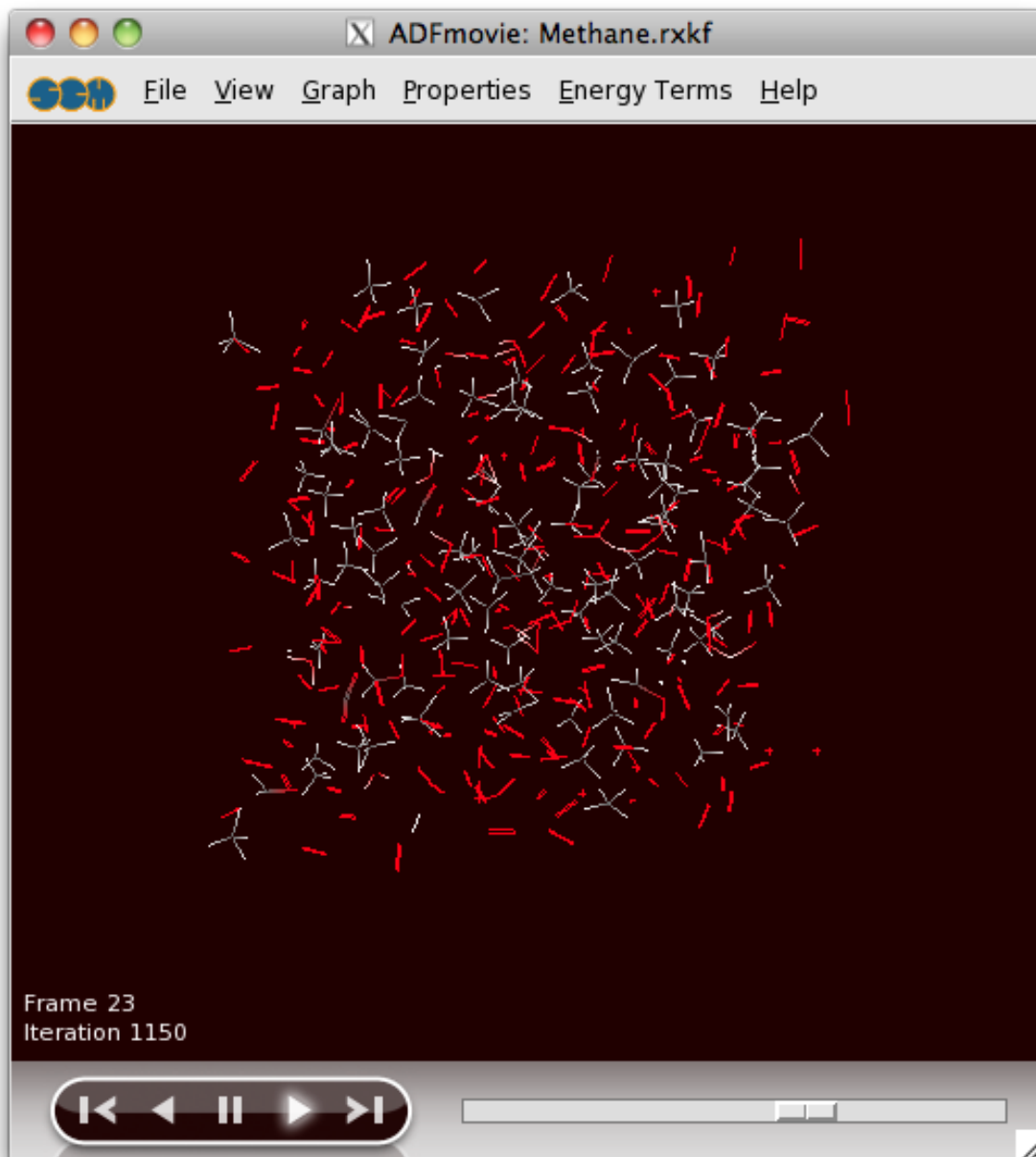
ADFjobs should come to the foreground, and your job should be visible at the top. On the right side you can see that the job is running (this is indicated by the gear-icon). When running, also a window will appear showing the progress of your simulation (the logfile):

Iteration	Nmol	Time(fs)	Epot(kcal)	Vol(A ³)	T(K)	Pres(MPa)	Dens(kg/dm ³)
0	306	0.00	-59564.53	15625.00	3500.00	0.00	1.03
50	349	12.50	-70618.30	15625.00	3804.21	0.00	1.03
100	351	25.00	-72616.07	15625.00	4348.15	0.00	1.03
150	349	37.50	-73568.30	15625.00	4565.73	0.00	1.03
200	342	50.00	-74099.05	15625.00	4632.91	0.00	1.03
250	348	62.50	-74278.30	15625.00	4598.70	0.00	1.03
300	346	75.00	-73313.74	15625.00	4222.96	0.00	1.03
350	354	87.50	-72273.61	15625.00	3865.79	0.00	1.03
400	344	100.00	-71254.15	15625.00	3449.83	0.00	1.03
450	348	112.50	-71959.45	15625.00	3651.62	0.00	1.03
500	349	125.00	-72782.40	15625.00	3880.13	0.00	1.03
550	339	137.50	-73615.65	15625.00	4120.46	0.00	1.03
600	345	150.00	-73590.92	15625.00	4073.29	0.00	1.03

As you can see in the logfile, the simulation is running.

To see more details, we now will use ADFmovie. Note that you can do this while the simulation is still running!

Start ADFmovie: **SCM** → **Movie** in the logfile window



ADFMovie will show you the trajectory of your system. Note that it will automatically read new data as soon as it becomes available.

It can also show graphs of the properties that ReaxFF calculates:

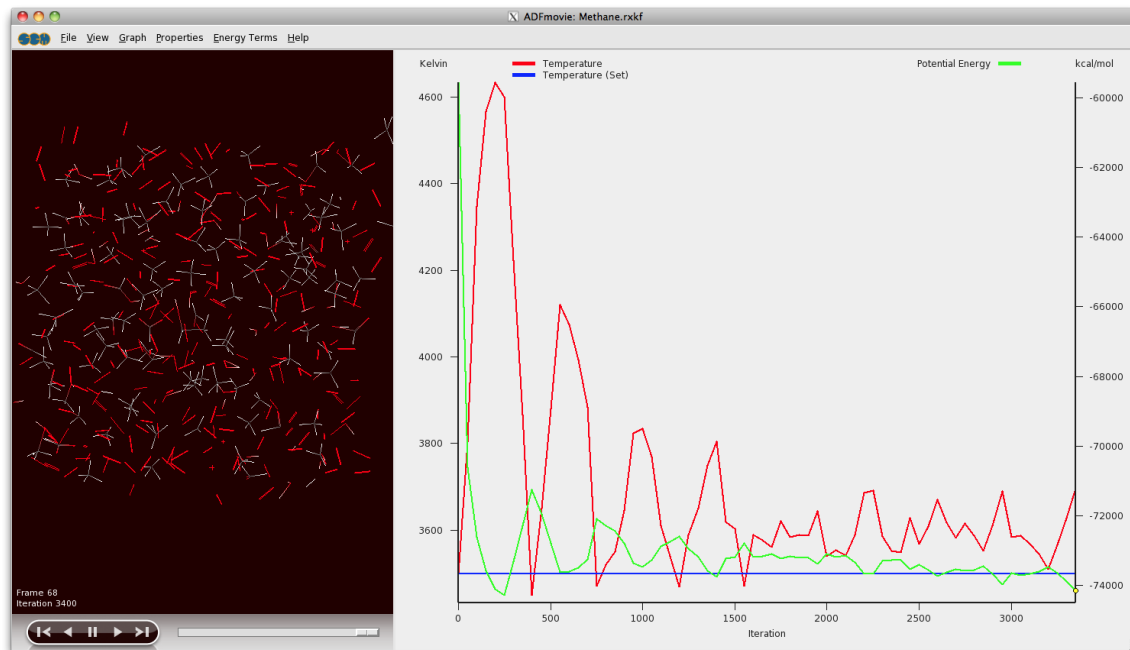
In the ADFMovie window:

Use the **Properties** → **Temperature** command

Use the **Properties** → **Temperature (Set)** command

Use the **Properties** → **Potential Energy** command

Make the window bigger to make viewing the graph easier



Note that the two temperatures (the actual temperature, and the set temperature) are both plotted on one axes. The other axes is used for the second property (in this case the potential energy).

You can go to a particular point in the simulation using the slider below the window showing your system, or you can click somewhere on one of the curves plotted. You can also use the arrow keys (left and right) to move through the simulation.

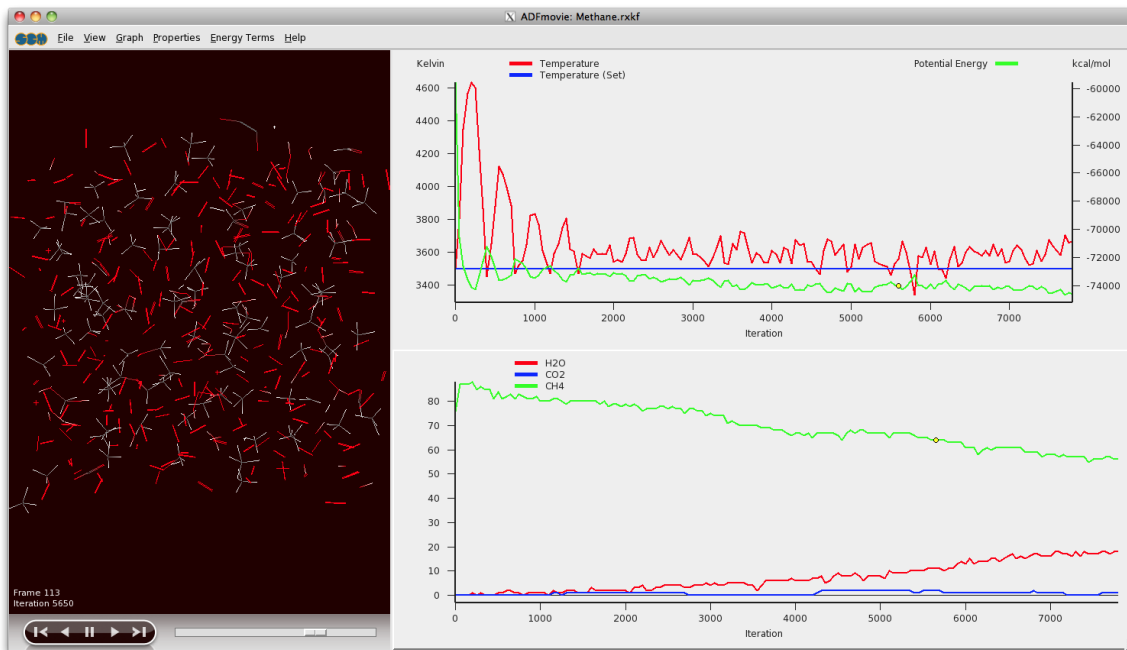
Click on the temperature curve

As ReaxFF is a reactive force field, reactions may take place. In this particular example the methane and ethanol should react with the oxygen, eventually producing H₂O and CO₂.

You can make graphs that show how many of the different molecule types are present. The following instructions often work, but it depends on what molecules are present in your simulation. You might try this step again after waiting some time. Especially the production of H₂O and CO₂ take some time.

Use the **Properties** → **Molecule Fractions** command
 In the window that pop-ups, select H₂O
 Click Add / Remove

Repeat these three steps for CO₂ and for CH₄

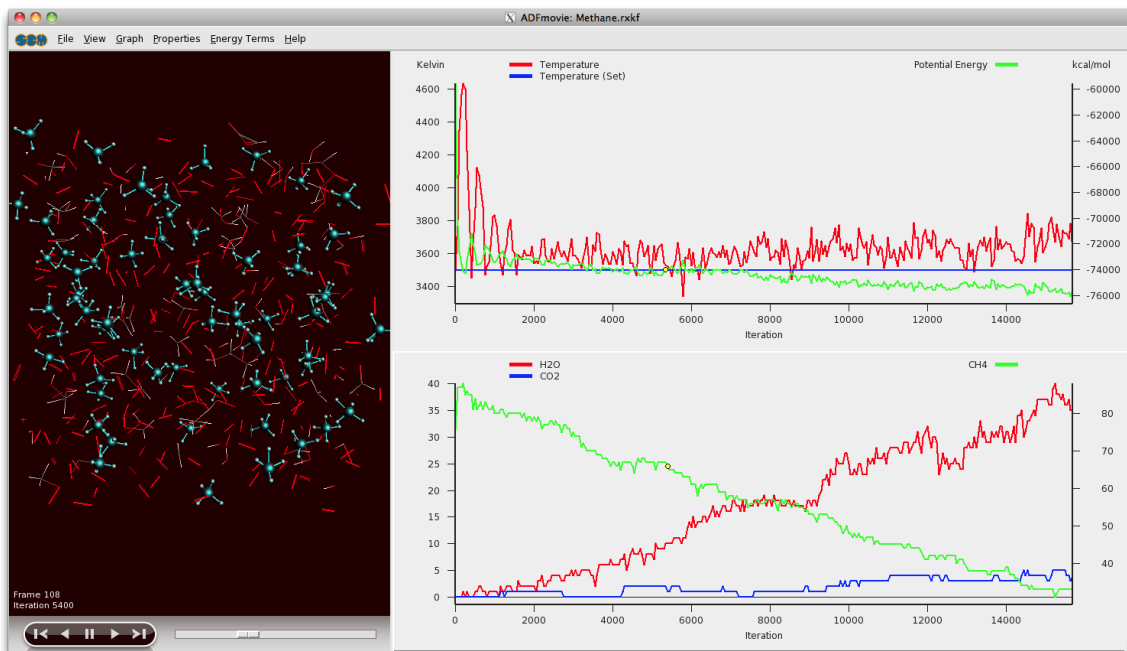


You can put one of the curves on a different axes if you wish:

Let the simulation run for some time

Click once on the curve showing the number of CH₄ molecules, this makes it the 'active' curve

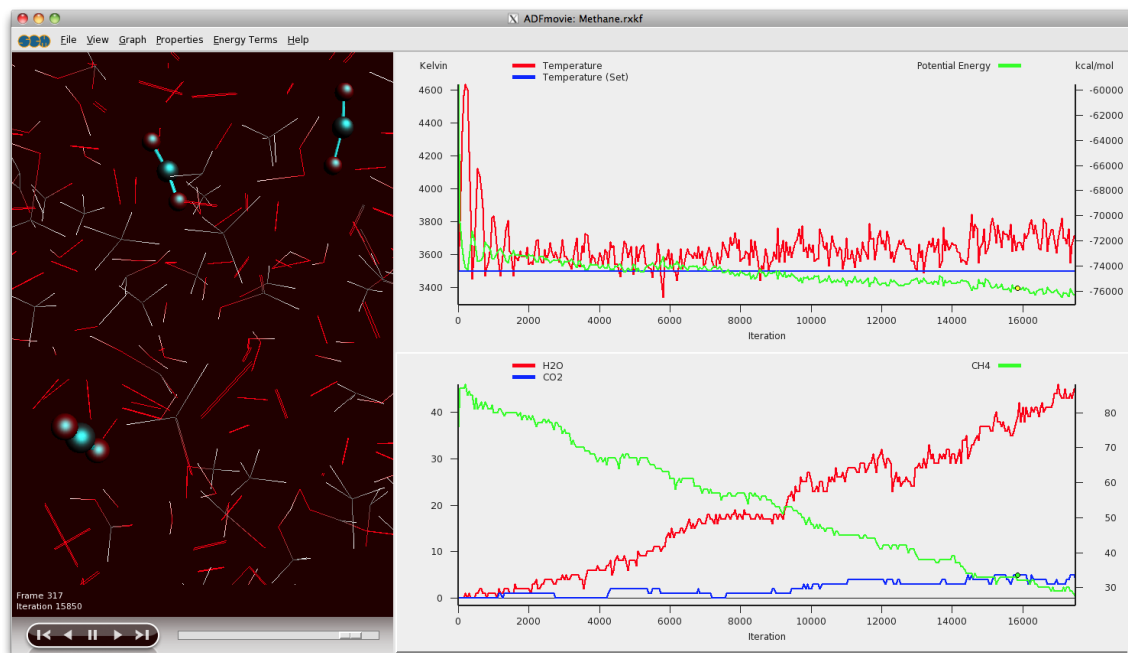
Use the **Graph** → **Curve On Right Axes** command



Clicking on the curve also had two other effects (besides making it the active curve): you jumped to the iteration in the movie corresponding to the point where you clicked, and the molecules that belonged to that curve are selected.

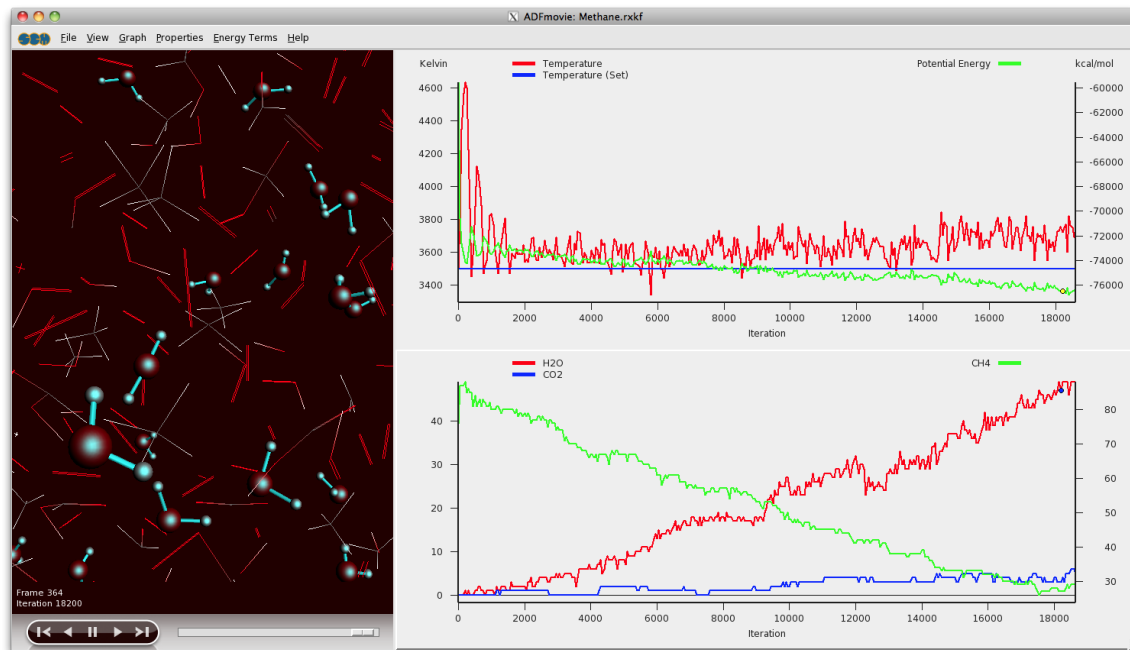
The selected molecules are shown with Balls and Sticks, instead of wireframe only, to make it easier to spot them. Flying to the selection also makes it easier to spot them:

Click on the curve showing the CO₂ production
Use the **View** → **Fly To Selection** command a few times



When you now go forward or backwards in time, it is easier to see how the reactions actually take place. Note that the atoms remain selected, even if they are no longer part of a CO₂ molecule. In a similar way you can focus on H₂O produced:

Click on the curve showing the H₂O production
Use the **View** → **Fly To Selection** command if needed



You can add additional curves for other molecules present, or for any of the energy terms calculated by ReaxFF. Just play around with it.

To prepare for the next tutorial, quit everything:

Bring the ADFjobs window to the foreground

If your job is still running:

select it

Job → Kill

Alternatively you can let it run to the end (40000 iterations) to see what happens.

Use the **SCM → Close** command to close all windows for this job

Tutorial 2: Water on an aluminum surface

This tutorial will help you to:

- create a slab using BANDinput
- import this slab in to ReaxFFinput
- add a solvent
- run the simulation and see what happens

Step 1: Preparations

Start ADFjobs

On a Unix-like system, enter the following command:

```
cd
adfjobs &
```

On Windows, one can start ADFjobs by double-clicking on the ADF-GUI icon on the Desktop:

```
Double click the ADF-GUI icon on the Desktop
```

On Macintosh, use the ADFLaunch program to start ADFjobs:

```
Double click on the ADFLaunch icon
```

Make a directory for the tutorial

We prefer to run the tutorial in a new, clean, directory. That way we will not interfere with other projects. Use ADFjobs to make the new directory:

```
Select the File → New Directory command (thus, the New Directory command from the File menu)
```

```
Rename the new directory by typing 'Tutorial2' and a Return
```

```
Change into that directory by clicking once on the folder icon in front of it
```

Start BANDinput

First we need to start BANDinput. We will use BANDinput to generate the Aluminum surface. Start BANDinput using the SCM menu:

```
Use the SCM → BAND input menu command
```

Step 2: Creating the surface

Bulk aluminum has an fcc crystal structure, with a lattice constant of about 4.0 Angstrom.

To create the surface, we first build bulk aluminum:

Use the Structure tool (the benzene like icon), and select the **Cubic → fcc** command

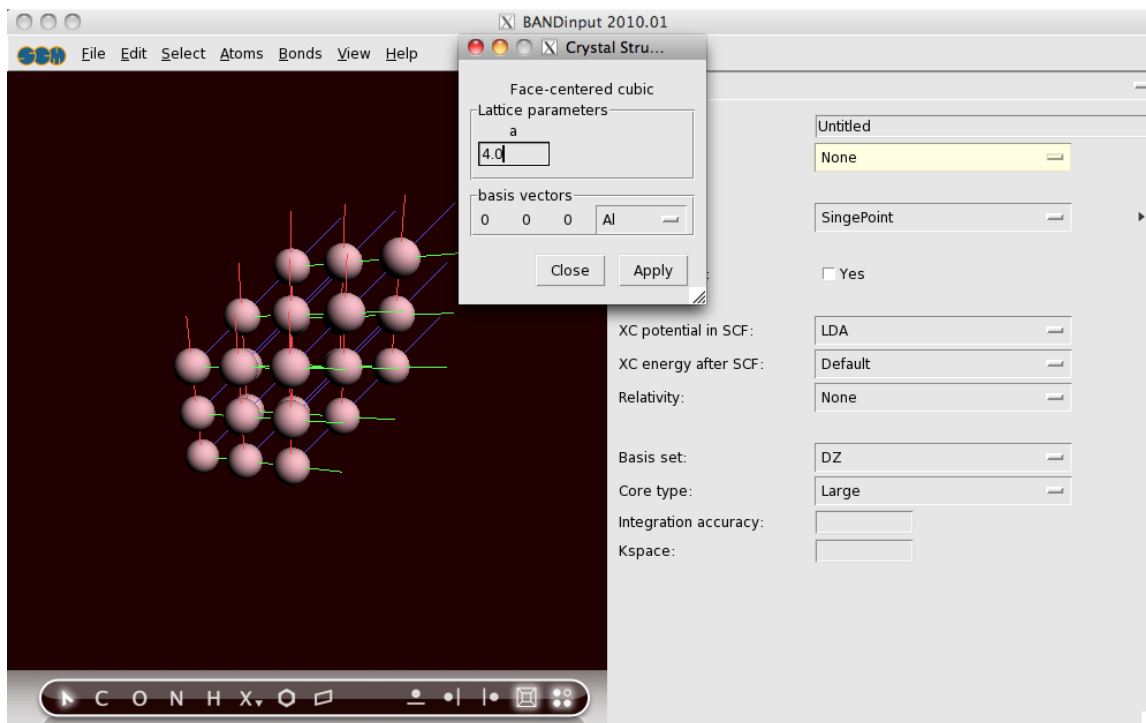
In the dialog that appears:

Set the lattice parameter to 4.0

Set the atom type to Al

Click the 'Apply' button

In your molecule editor screen you should see a picture of the bulk aluminum structure. The unit cell contains one atom, and by default BANDinput shows the unit cell repeated in all directions once.



Now create the surface:

Click the 'Close' button in the dialog that is still present

Click the 'Slice' tool (the button next to the structure tool)

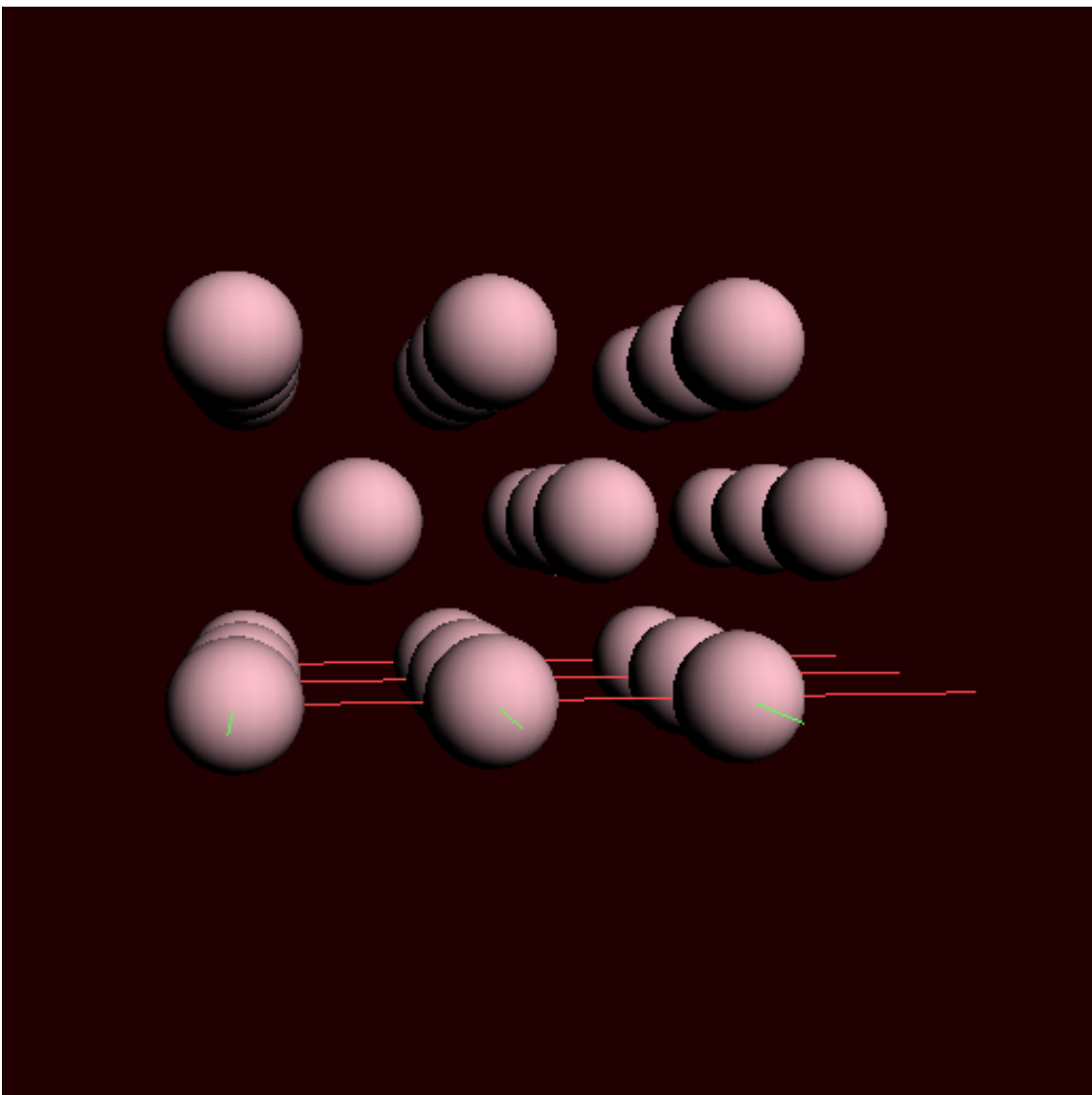
In the Surface Slice Tool dialog:

Check the 'cartesian' checkbox

Set the number of layers to 3

Click OK

Rotate the image to verify that you have a three-layer slice



Now we will copy this layer into ReaxFFinput:

Select → **Select All**

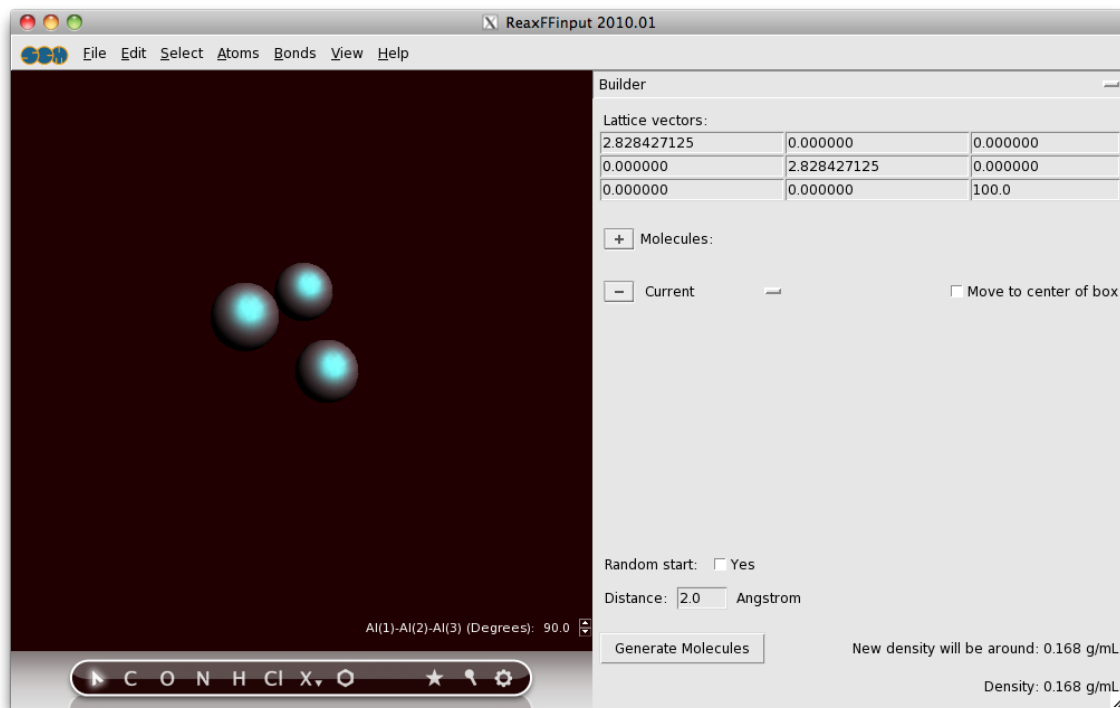
Edit → **Copy**

SCM → **ReaxFF input**

Edit → **Paste**

Rotate a little to verify three atoms are present

Select the 'Builder' panel



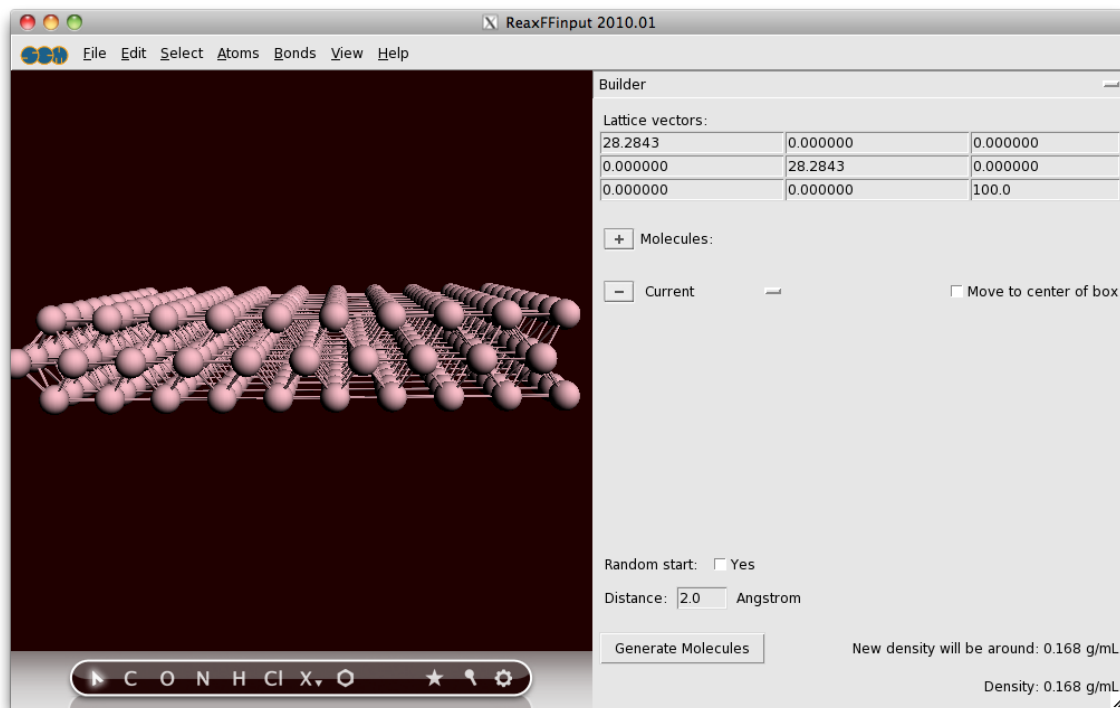
The unit cell for the aluminum layer has been copied to ReaxFFinput, and as you can see in the Builder panel the lattice vectors have also been adjusted properly. However, in this case we do not want just one unit cell, but a much bigger piece of the slab:

Edit → Generate Super Cell...

Put 10, 10, 1 on the diagonal

Click OK

Move around to get a better view

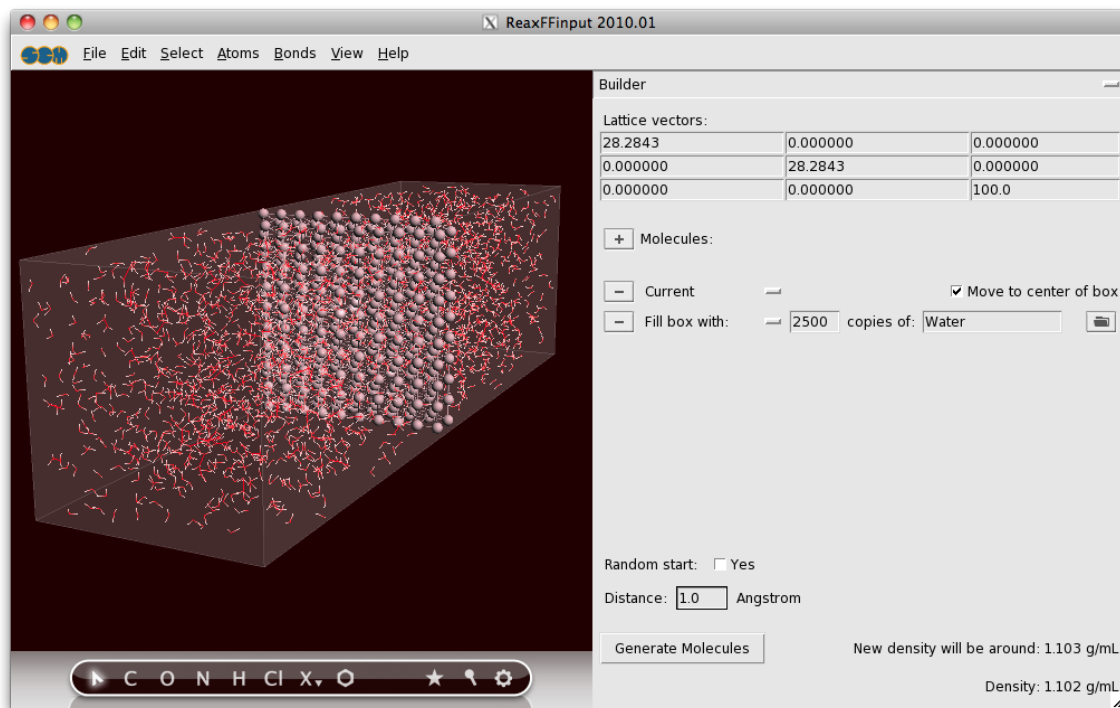


Now we have a real slab of aluminum, three layers thick. Note that the Generate Super Cell command adjusted the lattice vectors to match the new unit cell.

Step 3: Add solvent

The next step is to add water to the system, and make sure that the slab is in the center of the simulation box:

Check the 'Move to center of box' box on the line for the Current molecule
 Click the + button in front of Molecules:
 Click the file select button (on the right side of the 'Fill box with:' line)
 Select 'Water.xyz' and click Open
 Specify 2500 copies
 Specify a distance of 1.0 Angstrom (this is the minimum distance between the molecules)
 Click the 'Generate Molecules' button on the bottom
 Use the **View** → **Show Unit Cell** command to visualize the box
 Rotate to your favorite view



Step 4: Set up the simulation, including a temperature regime

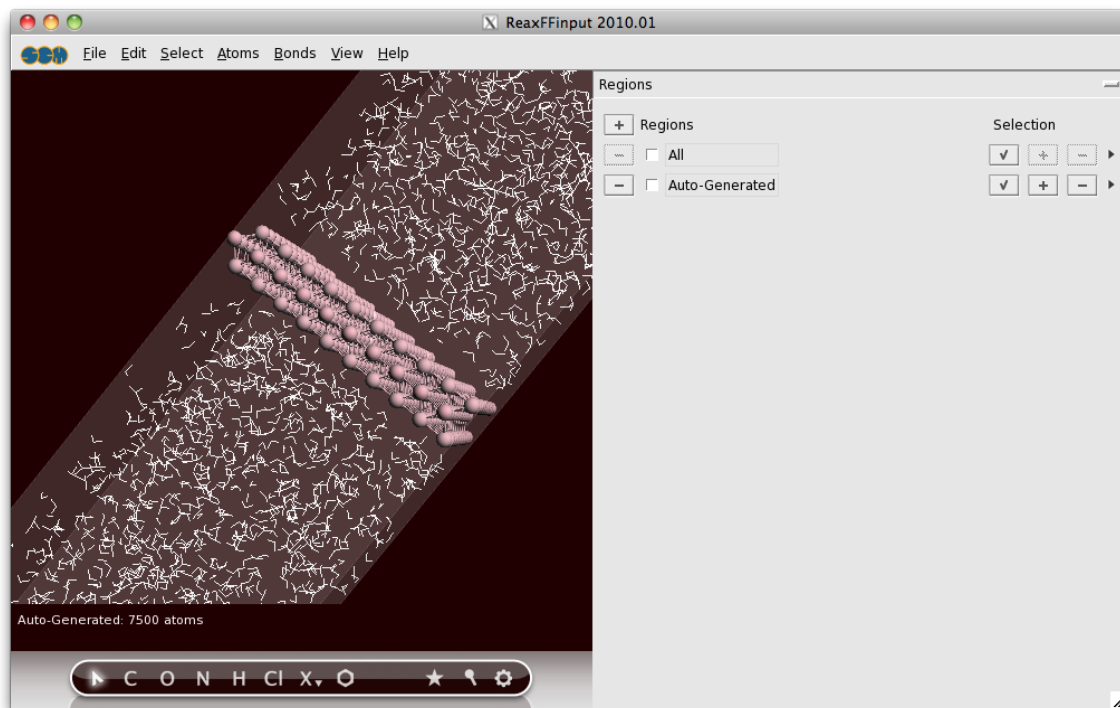
Now we will set up the MD-simulation. We will use the Al-water force field included in the undocumented directory:

```
Select the 'Main Options' panel
Select the 'Molecular Dynamics' Task
Click on the folder icon to select a force field
In the file select box, go into the undocumented folder
Select Al-water.ff
Click Open
Specify 100000 iterations
```

In the simulation we would like something to happen. So we will use a high temperature for water, but try to keep the aluminum cool. Also, we will start with a low temperature MD to relax the initial set-up. This can all be accomplished using a temperature regime, specifying different temperatures for different regions.

For this we first need to define two new regions: one for the aluminum slab, and one for the water. Regions in ReaxFFinput are the same as in the ADF-GUI: they are defined as a collection of atoms. Via the Regions panel you can define the regions:

```
Go to the Regions panel
Click once on the select button (the V like button) in the Auto-Generated region
Rotate and zoom to get a good view
```

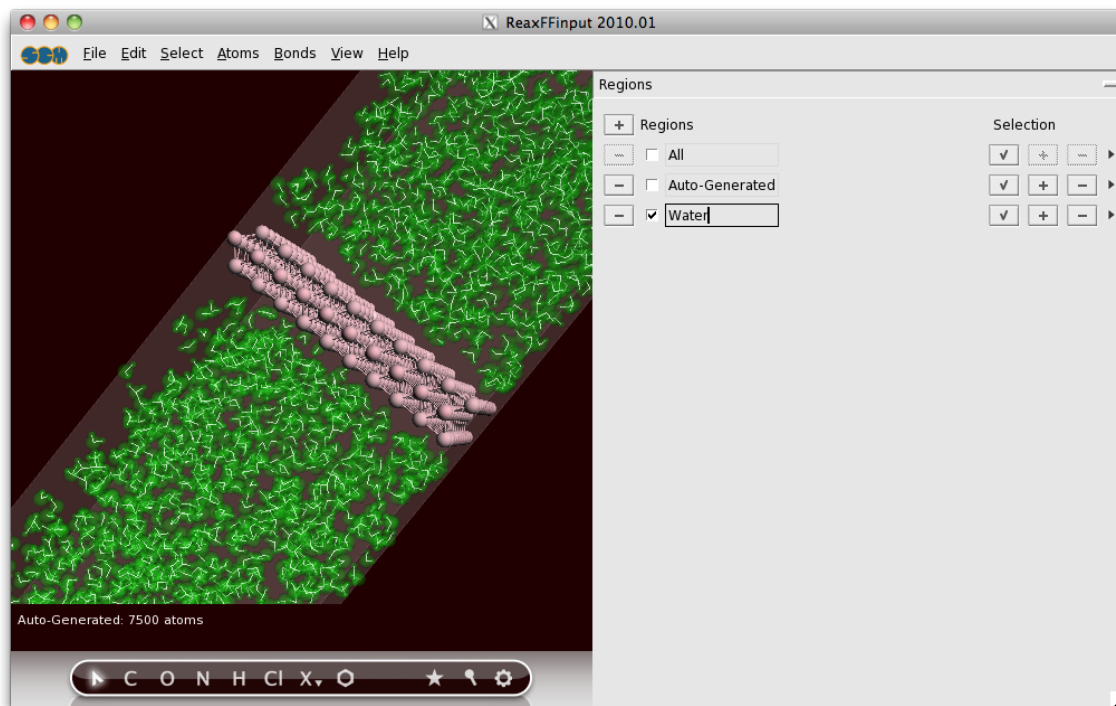


By pressing the select button you have selected all atoms in the 'Auto-Generated' region. This region will always contain the atoms that are added by the Builder. Thus, as you can see, all water molecules are selected.

We are going to set up a region for the water molecules, and a region for the aluminum surface:

With the water molecules still selected, press the + button in front of the Regions label

Click and select the text 'Region_2' and change it into 'Water'



Now we have a region defined that contains all water molecules. Note that the selected atoms (in this case all water molecules) were automatically added to the new region. The + and - buttons add or remove the selected atoms to a region.

Select → Select All

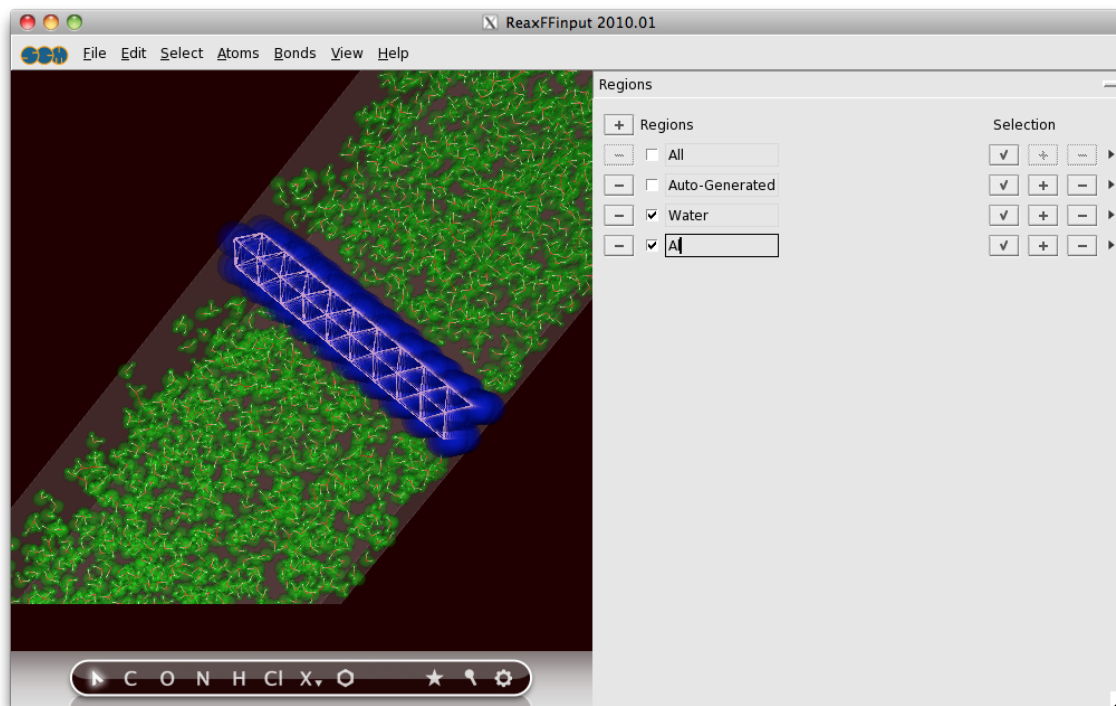
Press the + button in front of the Regions label again to add a new region (containing everything as everything was selected)

Change the name Region_3 to Al

Click the select button in the Water region to select all water molecules

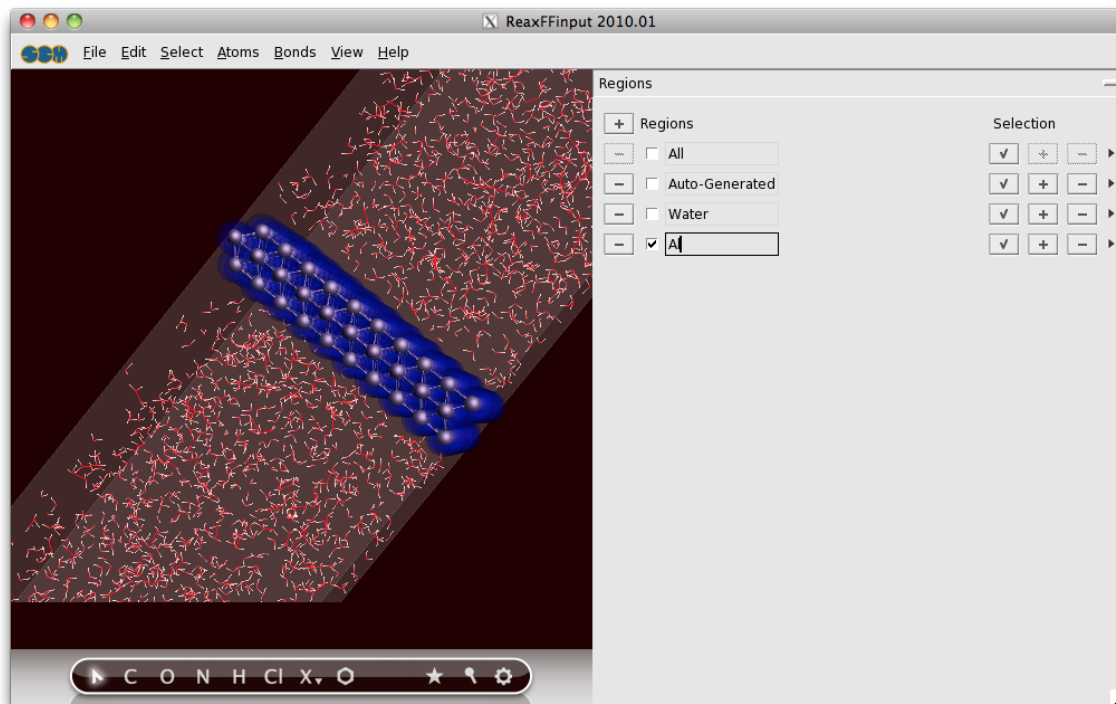
Click the '-' button in the Al region to remove the water from the Al region

Click in empty space to clear the selection



The different regions are shown with colors. This does make the display a lot slower. You can turn off (or on) this display with the check box in front of the Region names, and you can set visualization style per region:

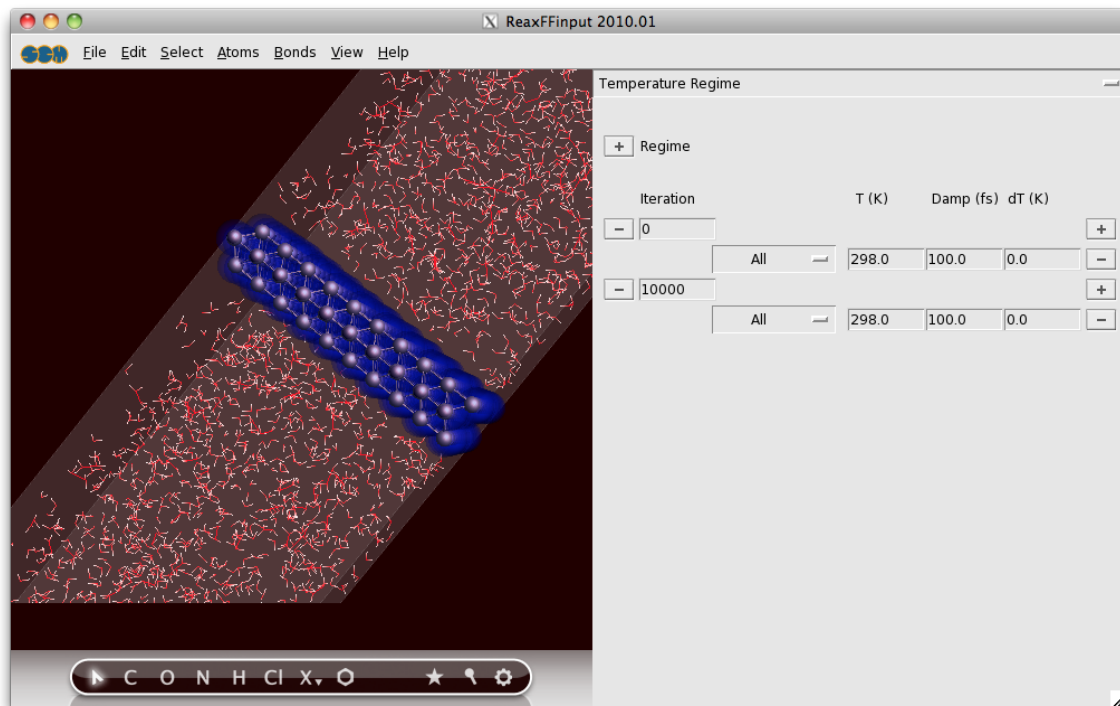
Uncheck the check box at the left of the Water region line
 Press the triangle on the right side of the A1 region line,
 and choose for the 'Balls And Sticks' visualization option



Now we have defined the regions that we need, now set up the temperature regime:

Select the 'Temperature Regime' panel

Press the '+' button in front of the Regime label twice to add two temperature steps



At iteration 0, we start with an MD simulation at T=0 K:

change the first 298 to 0 (note this applies to region All which is everything)

At iteration 20000, we set the water temperature to 2000, while keeping the aluminum temperature at 0:

Change the 10000 to 20000

Press the + button on the right side of the line starting with 20000

Change the first All on the 20000 step to Al, and change its temperature to 0

Change the second All on the 20000 step to Water, and change its temperature to 2000

Your temperature regime setup should look like this:

Temperature Regime

+ Regime

Iteration		T (K)	Damp (fs)	dT (K)
- 0	All	0.0	100.0	0.0
- 20000	Al	0.0	100.0	0.0
	Water	2000.0	100.0	0.0

Step 5: Run the simulation

Now we can run our set up:

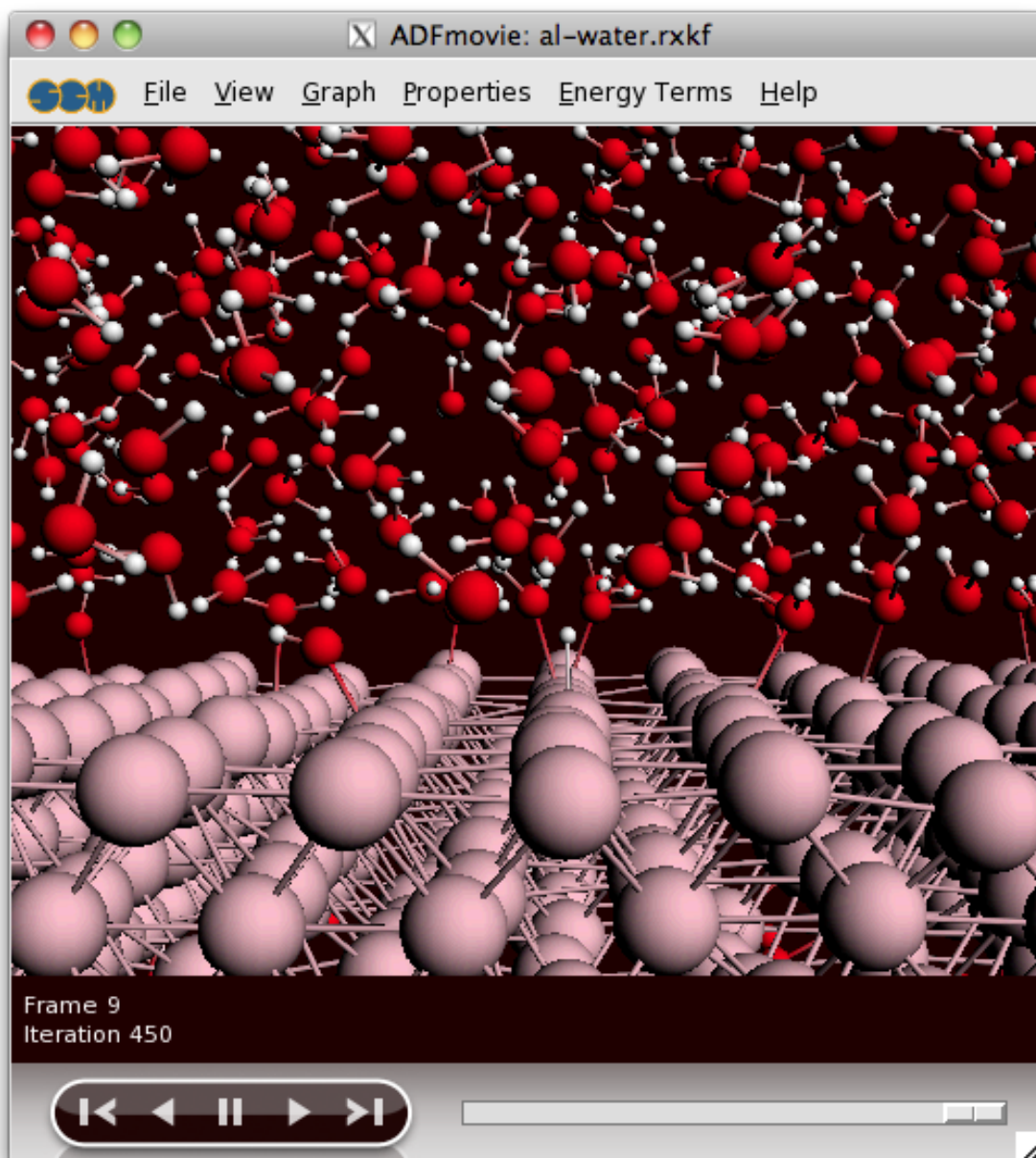
File → **Run**

When asked to save, specify Al-water as filename

Let it run for some time (until iteration 500 or so)

SCM → **Movie**

View → **Molecule Ball & Sticks** → **Balls And Sticks**



If you look around, you will most likely see many water molecules attaching to the aluminum surface. After some time, you might also see hydrogen atoms distracted from the water molecules, which are now moving around the surface on their own.

You might leave the simulation running to see what will happen. It will take a lot of time though.

If you do not want to wait for the simulation to finish, kill the job:

```
Bring the ADFjobs window to the front
Make sure your Al-water job is selected (click once on it if not)
Kill it Job → Kill
```

```
Close all GUI modules: SCM → Close All
```