



Scientific Computing & Modelling

ReaxFF Reference Manual

**ADF Program System
Release 2010**

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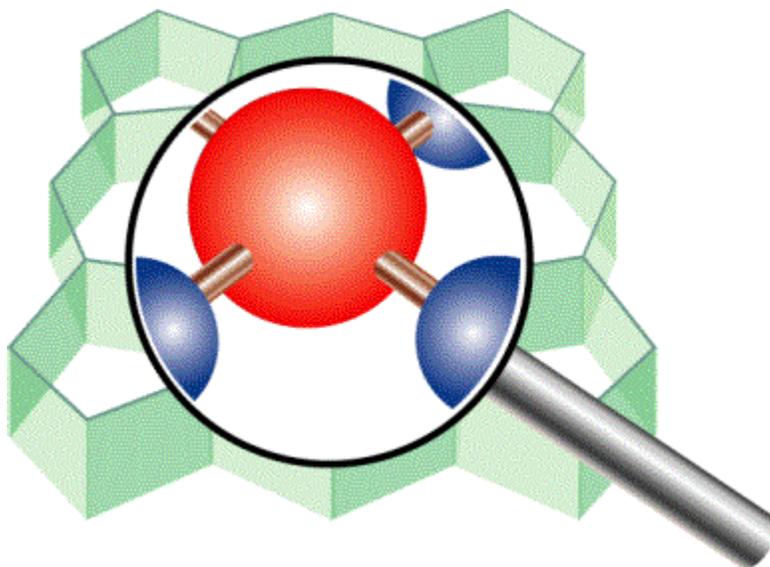


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ReaxFF: Molecular Dynamics using a Reactive Force Field

ReaxFF is a program originally written by Adri van Duin that performs Molecular Dynamics using a reactive force field. This version has been improved by SCM with regards to speed and memory usage, and a graphical user interface has been added.

As ReaxFF uses a force field, it is much faster in calculating energies and forces than a full quantum mechanical (QM) method. The special feature of the Reactive force field is that reactions may occur during the simulation. The changing atom types and connectivity is handled properly.

Like other force fields, the ReaxFF force field depends on many parameters. The quality of the results depend on how well the force field has been optimized for the kind of systems you are studying. The additional complexity of the reactive force field makes it slower than standard (non-reactive) force fields.

The GUI (graphical user interface) for ReaxFF is based on ADFinput. The tools in the GUI to create your system, and edit molecules are identical in ReaxFFinput and in ADFinput. However, ReaxFFinput has a special Builder panel that makes it easy for you to build large systems consisting of many molecules. This builder uses [Packmol](#) to build the actual system. Finally, ReaxFFinput allows you to set the main input options of your simulation.

Running your job is most conveniently done via ADFjobs. It will allow you to run on either a local or a remote system, and it will take care to move files to and from remote systems as required. While your job is running, the progress can easily be monitored.

When your simulation is ready, you can visualize the results using ADFmovie. It can show the trajectory of your system, and you can make graphs of most properties that ReaxFF has calculated.

SCM ReaxFF: what has changed

The SCM ReaxFF program is based on the original ReaxFF software as written by Adri van Duin. Many things have been changed, but we have tried to keep the new version compatible with the old one.

The main changes are:

- It has been optimized for speed
- It is running in parallel
- It has been optimized to reduce memory usage
- Many bugs have been fixed
- A new result file has been added (the .rxkf file) that contains all result and restart information
- A GUI has been added for both setting up your calculation (ReaxFFinput) and displaying results (ADFmovie)

Currently most of the old style result files can still be generated. The default values in ReaxFFinput are such that these old-style files are virtually never updated. The reason is that the new .rxkf result file is much more efficient, both in terms of writing and in terms of disk space needed. And it is much easier to access data from this file. The old style result files will not be maintained.

ReaxFF

Force Field

At the center of the ReaxFF-potential lies a bond order/bond energy relationship. Bond orders are obtained from interatomic distances and are continually updated at every iteration, thus allowing for connectivity changes. These bond orders are incorporated in all valence terms (i.e. energy contributions dependent on connectivity, like valence angle and torsion angle energy) ensuring that energies and forces associated with these terms go to zero upon dissociation. Furthermore, ReaxFF describes non-bonded interactions between all atoms, irrespective of connectivity. Excessive short-range repulsive/attractive non-bonded interactions are circumvented by inclusion of a shielding term in the van der Waals and Coulomb interaction.

For a more detailed description of the ReaxFF energy description see the original [ReaxFF manual](#).

ReaxFF aims to provide a transferable potential, applicable to a wide range of chemical environments. To ensure its transferability, the following general guidelines have been adopted in its development:

- No discontinuities in energy or forces, even during reactions.
- Each element is described by just one force field atom type. The ReaxFF metal oxide oxygen is described by the same parameters as the ReaxFF oxygen in organic molecules. ReaxFF does not have separate sp² and sp³ atoms for carbon, the method determines the atoms hybridization from its chemical environment.
- No pre-definition of reactive sites is necessary: given the right temperature and chemical environment reactions will happen automatically.

As the SCM ReaxFF program is compatible with the original ReaxFF program, please have a look at the original [ReaxFF manual](#) for a detailed description of many of the options. Note that the original manual is quite old, and some parts are no longer accurate.

Available Force Fields

In the ReaxFFinput main options panel, click on the 'i' on the right side of the Force field line. This will show a detailed description of the included force fields. This information is stored in the Readme file in the ADFHOME/atomicdata/ForceFields/ReaxFF directory.

At this moment, force fields are available for Ammonia Borane, AuO, Hydrocarbon oxidation, FeOCH, RDX/High energy, VOCH, and ZnOH. We will try to add more in the future.

Force Field optimization

In many cases you will need to optimize the force field (or even create a new one). For information on how to do this, see the original [ReaxFF manual](#).

There is no GUI support for force field optimization.

ReaxFFinput

Start ReaxFFinput

The ReaxFFinput executable is located in your \$ADFBIN directory. You can start it from the command line using:

```
$ADFBIN/reaxffinput
```

Alternatively, you can start it via the SCM menu in any of the ADF-GUI, BAND-GUI or ReaxFF-GUI programs.

After starting ReaxFFinput you will see the two main parts: on the left side is the drawing area where you construct your molecules, and on the right side are panels that allow you to set the simulation options.

Molecule Editor

The molecule editor on the left is identical to the editor that is used for ADF. Please check the [ADF-GUI reference manual](#) for details. It might also be a good idea to try the some of the [ADF-GUI tutorials](#), especially tutorial 1 and 4.

One special feature to mention: you can copy and paste molecules between the different GUI modules, including lattice constants. Thus if you build a slab using BANDinput, you can select that and copy it to ReaxFFinput. Not only will you get the slab, but also the lattice vectors will be adjusted properly. An example of this can be found in the second [ReaxFF tutorial](#).

Builder

On the right are the input panels. One of the panels is special: it is not really an input panel, but gives access to the builder. To get that panel, use the pull-down menu on top of the panels and select Builder.

The Builder allows you to compose your system of many replicas of some predefined molecules. These molecules are replicated as often as you want, giving a simulation box full with these molecules. Thus it is very easy to generate a liquid or a gas.

First, however, you need to define your simulation box. ReaxFF performs all simulations using periodic boundary conditions. In the Builder panel you define the lattice vectors that define the unit cell. The default is a box with sides of 25 Angstrom.

Next is the part where you define what molecules to add to your system. Press the + button to add more molecules, or press the - button in front of a line to remove that particular molecule.

The 'Current' option will include whatever you have manually created on the left side. For example, some molecules to be solvated. Or some slab imported from BANDinput.

The 'Fill box with' option allows you to select what molecule to use for filling. The geometry of the molecule must be available in a file with .xyz extension, and it should contain the coordinates and atom types of your molecule in XYZ format. Many typical molecules are included with ReaxFFinput. When you press the folder button at the right side you will be able to select your molecule via a file-select browser.

As you may have more than one kind of molecule, you can also make mixtures of different molecules.

Once you press the 'Generate Molecules' button, the actual packing of the molecules is done using [Packmol](#).

If you find using the Builder useful, please give proper credit via the following reference:

L. Martínez, R. Andrade, E. G. Birgin, J. M. Martínez. Packmol: A package for building initial configurations for molecular dynamics simulations. *Journal of Computational Chemistry*, 30(13):2157–2164, 2009.

Input Options

The panels on the right side allow you to set your simulation options (that is, to set the ReaxFF input options). Most options should be self-explaining. If you hold your mouse over one of the options without moving, a balloon will pop up with a descriptive text that should explain what that option is for.

Running your job

ADFjobs

You can run your set up using the Run command in the File menu of ReaxFFinput. This will use ADFjobs to run the job. You can run on your local machine, or you can have your job being sent to some remote machine.

Please see the [ADF-GUI reference manual](#) for further details.

ADFmovie

You can examine the results of your ReaxFF simulation using ADFmovie. This works both when the calculation is finished, and while the calculation is still running. It also works when your job is running on a remote machine through ADFjobs: ADFmovie will automatically fetch the data it needs to visualize. Note that this is typically much less data than the full result file.

Via the menus in ADFmovie you can visualize the different thermodynamic terms that ReaxFF calculates, as well as the different energy terms. Using the 'Molecule Fractions' command in ADFview you can also make plots of the number of different molecules present. This is very convenient for following reactions.

For a detailed description of ADFmovie, see the [ADF-GUI reference manual](#).