AutoIMD User's Guide

AutoIMD version 1.7

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Contents

1   Introduction to AutoIMD

AutoIMD is a means of quickly starting a NAMD molecular dynamics simulations from atomic coordinates in VMD. The simulation can then be visualized in real-time on the VMD graphics screen. With the appropriate devices (such as a VRPN tracker), the user can also interact with a running simulation and apply forces to individual atoms or residues. Such an interaction is extremely useful when building and modeling systems, and can also be used to gain precious insights by tinkering with key residues and atoms.

While the *Interactive Molecular Dynamics* (IMD) technology that enables all of this is an intrinsic part of VMD, AutoIMD makes it much more accessible and useful. In general terms, AutoIMD adds the following capabilities:

- The user can instantaneously get a simulation running for a subset of his/her system which is specified through a VMD atom selection.

- Instead of a full-blown simulation, AutoIMD can also be used to quickly minimize the energies of parts of a system (*e.g.*: on which external manipulations have been performed, for example).

- It provides a graphical user interface for setting basic simulation parameters as well as for specifying which machine or cluster to run the simulation on.
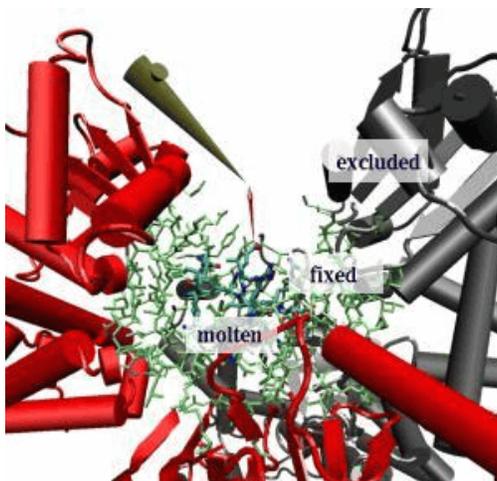

Figure 1: An example AutoIMD session. The molten zone is in the center, surrounded by the fixed zone and then by the excluded zone. A pointer is being used to interact with the system in real-time.

Fig. 1 is an example of an AutoIMD session. When using AutoIMD, you can divide up your system into three distinct regions, shown in the figure:[1]

- The *molten zone* is the region where the atoms are allowed to move freely, typically surrounded on all sides by the fixed zone. This is the part of the system that you are interested in interacting with (typically using a *pointer* as shown). You can refer to this region through the `imdmolten` atomselect macro.

- The *fixed zone* is included in the simulation, but its atoms are held fixed. Forces from atoms in the fixed zone will affect the moving atoms and constrain their motion. You can refer to this region through the `imdfixed` macro.

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[1] The "molten zone" method used here was first discussed in the context of IMD in J. Prins et al. A virtual environment for steered molecular dynamics. *Future Generation Computer Systems* **15**, 485–495 (1999).

- The *excluded zone* is removed from your system before the simulation is started and are ignored by the simulation (in order to speed it up). You can refer to this region through the `imdexcluded` macro.

2   AutoIMD Requirements

To get started using AutoIMD with your system, you will need the following:

1. A computer running VMD. Computers running MS Windows are supported as of VMD 1.8.4.

2. An installed copy of NAMD, preferably in the default path `/usr/local/bin` (if not, you will get a prompt). If you wish to run your simulations on a local cluster, you need to perform some additional steps which are detailed later, in section 5.

3. If you wish to use a haptic device, you must also set up VMD accordingly (see the VMD documentation).

4. Atomic coordinates (from a PDB, DCD file, etc.) and a PSF file describing your system.

5. A CHARMM parameter file for your simulation if your system requires non-standard parameters. The standard parameters are included in AutoIMD, but can also be downloaded here:
http://www.pharmacy.umaryland.edu/faculty/amackere/force_fields.htm.

3   How to Run an AutoIMD session

1. Start VMD, load your system (make sure to include a PSF file), and start AutoIMD from the **Extensions → autoimd** menu item (in the VMD main window). The AutoIMD window (Fig. 2) should appear.
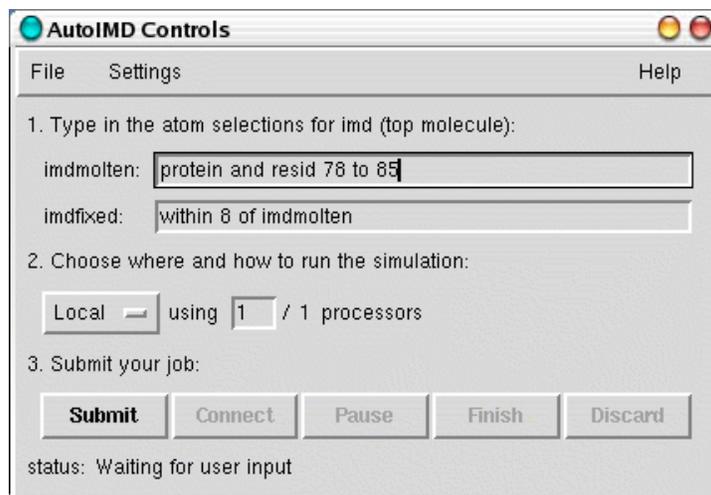
Figure 2: The AutoIMD main window.

2. *[OPTIONAL]* Select the **Settings→Simulation Parameters...** menu item from the AutoIMD window. The dialog box shown in Fig. 3 should pop up. Use this dialog box to tell AutoIMD the location of your scratch directory. You may also specify an alternate set of CHARMM parameter files, if your system contains non-standard residues.

3. Specify the molten zone by entering a VMD atom selection into the text box.
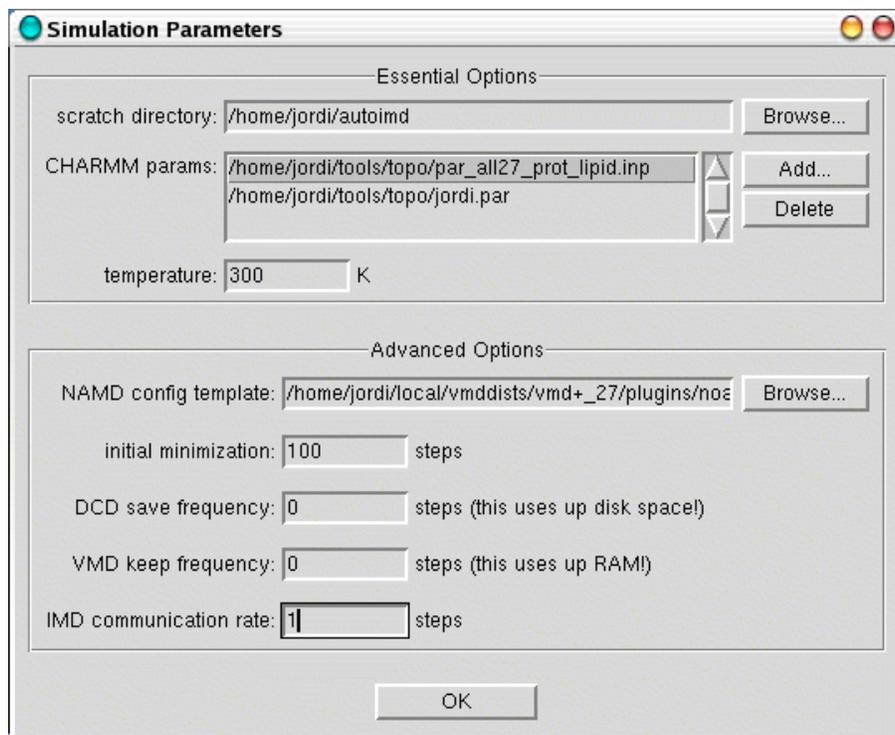
Figure 3: The AutoIMD Simulation Parameters dialog box.

NOTE: Because of the way that AutoIMD currently works, you should avoid referencing atoms by their `index` *or* `residue` *number (since they will change in the simulated system), instead, refer to atoms using their* `name`, `resid` *and* `segname` *or* `chain`, *etc.*

4. Optionally, you can also change the fixed zone that is used to hold the molten zone into place, although the default should work. Note that the fixed zone that you specify might later be adjusted by AutoIMD to include complete residues instead of residue fragments, this is normal.

5. Pick a server and adjust the number of processors. If you want to run the simulation on the same computer that VMD is running on, you would pick "Local" and ignore the processors field.

6. Click the **Submit** button to start your NAMD simulation.

NOTE: If this is your first time running AutoIMD, it will prompt you to create a scratch directory in which AutoIMD will store its temporary files. The scratch directory needs to be accessible on both your local machine and the host on which NAMD will run. Do not store your own files in this directory.

NOTE: If you get an error message saying "Unable to open psf file xxx.psf.", you need to reload your PSF file on top of your current molecule one more time and click Submit again.

7. Click **Connect** to connect to the simulation with IMD. You should see the atoms start to move.

NOTE: It might take a few seconds for the NAMD simulation to get started. During this time, VMD will not be able to connect and you will see some error messages of the type: Error connecting to host on port xxxx. This is normal, and these errors can usually be ignored. VMD will connect as soon as NAMD is ready.

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NOTE: If after waiting a long time, AutoIMD still does not connect, your simulation may have had trouble starting properly. Make sure that your simulation is actually running. If not, your NAMD job may have aborted. Check the NAMD output in the autoimd.log file in your scratch directory to find the reason (NAMD will say there why it crashed, etc.). Once this is fixed, you can click on Discard and then Submit, to try again.

8. Interact with your system for a while. You can use the **Mouse → Force** menu items, or a 3D tracker to pull on your atoms. Alternatively, just can also just watch your system equilibrate. At any point during your simulation, you can save a PDB snapshot of your system by choosing the **File → Save Full PDB As...** menu item.

9. When you are done, click **Finish**. The coordinates of your atoms in your originally loaded molecule will updated, and the simulation will stop. **Discard** also stops the simulation, but does not update the coordinates and you will be brought back to your initial state. Use this button it if anything goes wrong.

4 AutoIMD Adjustable Parameters

AutoIMD allows you to set a number of adjustable parameters, through the Simulation Parameters window (**Settings → Simulation Parameters** menu item). These options are described here:

scratch directory   The directory in which AutoIMD will store its temporary files needed to run the NAMD simulation. Do not store your own files it it.

CHARMM params   The list of CHARMM parameters files used by NAMD. You will need to modify this if your system contains non-standard residues for which you have created parameters.

temperature   - The temperature at which the simulation dynamics will be run, in degrees Kelvin.

NAMD config template   - AutoIMD runs a NAMD simulation using a pre-defined template which contains all the instructions to be followed by NAMD. If you wish to create a custom simulation, e.g. use different NAMD settings and protocols than what AutoIMD offers, you should copy the template provided by AutoIMD, edit it, and specify it here.

initial minimization   The number of minimization steps performed before the equilibration starts.

DCD save frequency   The frequency at which simulation steps are saved to disk. These will be located in a DCD file called autoimd.dcd in the scratch directory. To load and view this trajectory in VMD, you will also need to load the autoimd.psf file in the same directory.

VMD keep frequency   The frequency at which simulation steps are kept in VMD's memory. You can view these by using the trajectory animation slider.

IMD communication rate   If this is set to something greater than 1, NAMD will not send every computed step to VMD, but will skip steps and only send coordinates to VMD at a set interval.

5 Making your settings permanent and adding new servers

If you use AutoIMD a lot, you might wish that could set your default settings in a startup script and not have to worry about typing them in each time. Almost everything in AutoIMD is customizable.

To set your default scratch directory and CHARMM parameter file, you can include the following lines (provided as an example only) in your `.vmdrc` startup file. Be sure to use absolute paths!

```
package require autoimd

autoimd set scratchdir  /home/user/scratchdir
autoimd set parfiles    {/home/par_paramfile1.inp  /home/par_paramfile2.inp  ...}
[...]
```

For more advanced customization, it is recommended that you copy the file `autoimd-settings.tcl` that is distributed with the AutoIMD package, to your local directory. You can then edit it to suit your needs (it is self-documented). Have it be run at startup by adding the following line to your `.vmdrc` file (be sure to use the right path):

```
source autoimd-settings.tcl
```

If you have access to a local cluster for running NAMD, this file is also where you would tell AutoIMD how to access it.

6 Customizing the representations used during AutoIMD

AutoIMD uses multiple representations to help you keep track of the molten, fixed, and excluded zones in your simulation. When a simulation is submitted, two molecules are used at once: one containing the original, complete structure and one containing just the atoms needed for IMD. To avoid showing the same atoms twice, AutoIMD displays only the excluded and fixed zone of the original molecule. To accomplish this, the atomselection macros `imdexclude`, `imdfixed`, and `imdmolten` are defined to correspond to the three regions of the simulation. You can take advantage of them to select desired parts of your simulations.

You can customize both molecules' representations with the VMD Graphics Form, just as in a normal VMD session. AutoIMD saves the representation used for the IMD molecule when ending a simulation and reloads it when a new simulation is submitted. The default IMD representation can be permanently customized through AutoIMD's `imdrep` variable. Here is an example of how it can be used:

```
autoimd set imdrep {
    mol representation Bonds 0.300000 6.000000
    mol color Name
    mol selection "imdmolten and not hydrogen and not water"
    mol material Opaque
    mol addrep $imdmol

    mol representation VDW 1.000000 8.000000
    mol color Name
    mol selection "imdmolten and numbonds 0"
    mol material Opaque
    mol addrep $imdmol

    mol representation Bonds 0.300000 6.000000
    mol color Name
```

```
    mol selection "imdmolten and water"
    mol material Opaque
    mol addrep $imdmol

    mol representation Tube 0.400000 6.000000
    mol color ColorID 12
    mol selection "imdfrozen"
    mol material Opaque
    mol addrep $imdmol
}
```

To view the current IMD representation, you would type (at the VMD prompt):

```
puts $AutoIMD::imdrep
```

7   Getting Additional Help

For additional help, as well as to provide feedback, contact us as `vmdks.uiuc.edu`.