Graphical User Interface to Run Molecular Dynamics Simulations of CNT-Polymer Hybrids in VMD

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Abstract

Carbon nanotube-Polymer (CNT-Polymer) hybrids have many useful properties important in the field of nanoscience. Actually they are difficulties when someone want to start doing MD simulations because this is a very complex process. This work aims to help all the people (the rookies and the experts) to work with MD simulations. The software used here was VMD, DrPython and script developed by us. The development of a GUI with a main menu and some windows was done. Each window has a special function for this application. This GUI is good tool for people who want to study the hybrid systems. The prototype of this GUI is proven to be a good tool to perform MD simulation of CNT-Polymer hybrids.

Keywords: Molecular Dynamics, DNA-CNT hybrids, VMD

1. Introduction

Molecular dynamics (MD) simulations are well-suited to provide insights into the fundamental properties of CNT-Polymer hybrids because they enable calculation of structural properties with atomic resolution. For example, ss-DNA-CNT hybrids have been recently used to construct nanoscale chemical sensors.

They are some problems when someone want to start doing MD simulations because this is a very complex process. This work pretends to help all the people (the rookies and the experts) to work with MD simulations. The work presented here is a Graphical User Interface (GUI) that is used like a VMD plugin to develop MD simulations.

2. Background

2.1 polymer classification

Basically we have two main groups of polymers: homopolymer and copolymer. The homopolymer is a polymer in which all the monomers are basically the same monomer. For example if we take the sequence of DNA: CCCCCCCCC, that is an homopolymer. The homopolymers available in this work are: Poly-CYT, Poly- ADE, Poly-GUA, Poly-THY, and Polyaniline. The other group is the copolymer, a copolymer is a polymer made with different monomers. And example of a DNA sequence of a copolymer is: GATGCCCAGT. In our work the copolymer available is the single strand DNA.

2.2 VMD

VMD is designed for the visualization and analysis of biological systems such as proteins, nucleic acids, etc. It may be used to view more general molecules, as VMD can read standard Protein Data Bank (PDB) files and display the contained structure. VMD provides a wide variety of methods for rendering and coloring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. VMD can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VMD can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer.

2.3 GUI

A graphical user interface or GUI is a type of user interface which allows people to interact with a computer and computer-controlled devices. Instead of offering only text menus, or requiring typed commands: graphical icons, visual indicators or special graphical elements called "widgets", are presented. Often the icons are used in conjunction with text, labels or text navigation to fully represent the information and actions available to a user. The actions are usually performed through direct manipulation of the graphical elements.

Every GUI needs basics considerations of usability like has to be quick to use and relatively error-free. It must do what the user wants. Usability means that the product does what you need it to do, it does that quickly and safety, and it is easy to learn.

3. Software and methods

The software used in this work were Visual Molecular Dynamics, DrPython and scripts developed by us. VMD is a very powerful program that can be use as an intermediary to run other software or scripts. All the code was written in DrPython using the libraries of Tkinter. Our scripts were also written in Pyhton. The work was done in a Linux operating system's machine.

4. Results

The development of a GUI with a main menu and some windows was done. Each window has a special function for this application.
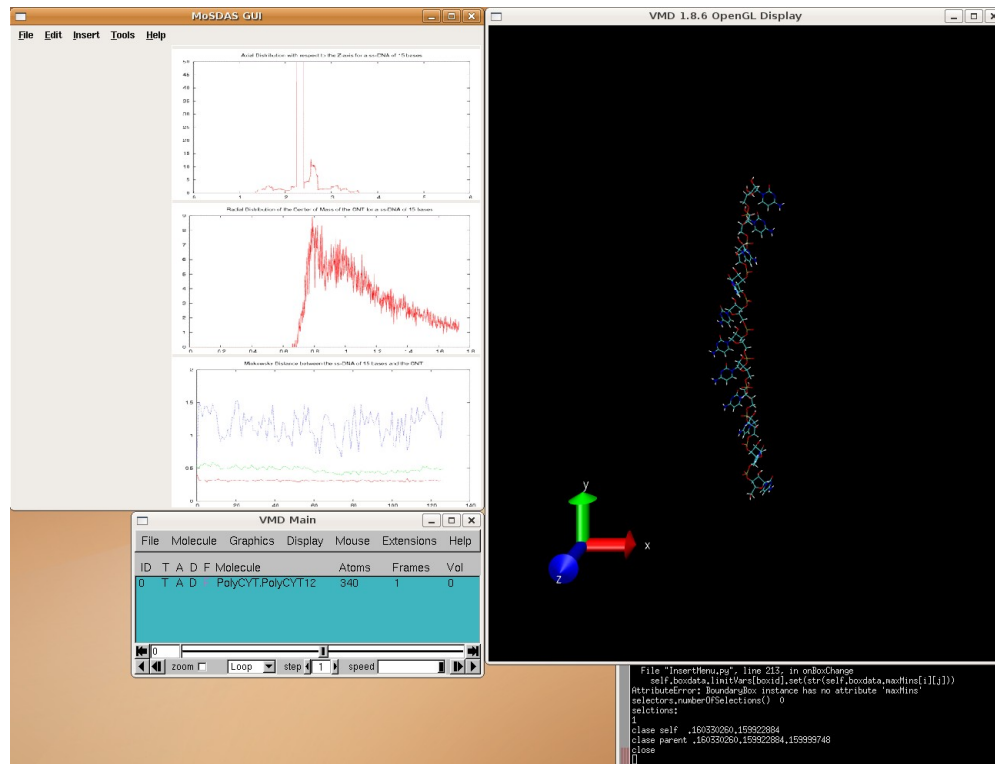
Figure 1 shows the actual state of the GUI.

Figure 1. Actual state of the GUI.

This GUI has four phases:

1. to set up the system that is going to be simulated
2. make the corresponding files to run the simulation
3. run the simulation
4. analyze the data when the simulation is running

4.1 Phase 1

The first thing to do is to insert a polymer and/or fiber to the system. To do that two different windows were created. Figure 2 shows the window for polymers and Figure 3 shows the window for fibers.
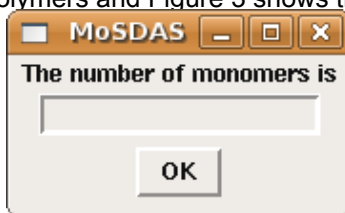

Figure 2. Window to insert a polymer.

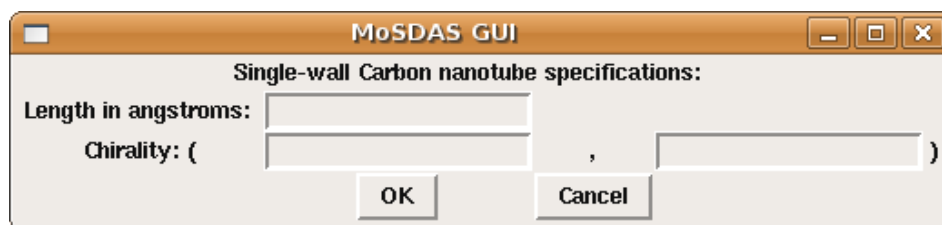This window needs the number of monomers to create the respective polymer.

Figure 3. Window to create a CNT.

To create a CNT you need to enter the length and the chirality of the tube.

Also at the first phase they are other windows that are essential to create the system. These windows are to select molecules, to insert a box, to move a molecule, and to merge two or more molecules.

The selection window is very important because you need to select first the molecules that you want to edit. Figure 4 shows that window.
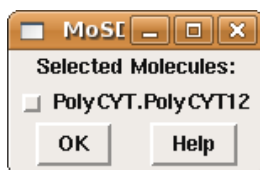

Figure 4. Selection window.

This window show the name of the molecules. Here for example the molecule inserted was a Poly Cytosine of 12 monomers. There is a radio button to select the molecule and the press OK.

The bounding box window have suggested values for the box. It also have the option to add the ratio cutting distances. It is show in the Figure 5.
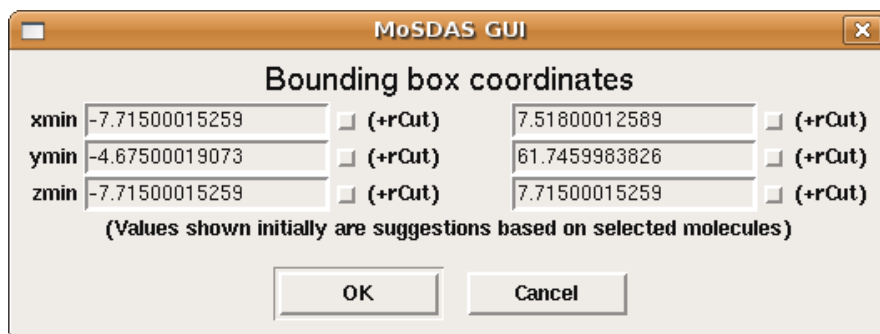
MoSDAS GUI

Bounding box coordinates

xmin	-7.71500015259	☐ (+rCut)	7.51800012589	☐ (+rCut)
ymin	-4.67500019073	☐ (+rCut)	61.7459983826	☐ (+rCut)
zmin	-7.71500015259	☐ (+rCut)	7.71500015259	☐ (+rCut)

(Values shown initially are suggestions based on selected molecules)

OK   Cancel

Figure 5. Bounding box window.

Also there are a move and a center the molecule windows. These windows are shown at Figures 6 and 7.

MoSDAS GUI

Displacements

X: [   ]   Y: [   ]   Z: [   ]

Move   Cancel   Help

Figure 6. Move the molecule window.

The input for this windows are the coordinates that you want to move the molecule.

MoSDAS GUI

Selected Molecules are:

CNT.CNT(10,10)

PolyCYT.PolyCYT12

Center these molecules?
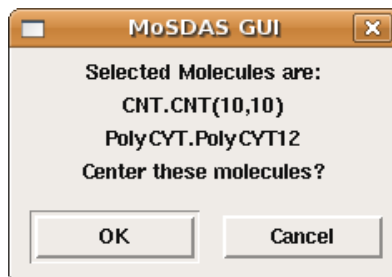
OK   Cancel

Figure 7. Center the molecule window.

This window shows the selected molecules and ask to the user if he want to center those molecules.

Next is the merge window. It's very useful because our goal is to have a system. So when we have more than one molecule, we use make a merge and then we have only one molecule that contain all the system. Figure 8 shows the merge window.
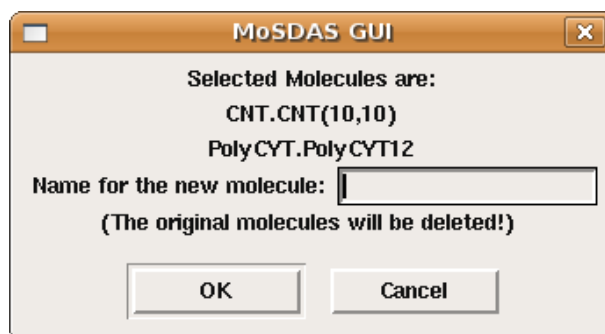

Figure 8. Merge window.

It has the names of the selected molecules and ask for the new name of the system.

After the system is ready we need to make the files, so then we can run the simulation.

4.2 Phase 2

We want to run the MD simulations with NAMD software this software need essential files to run the simulation.

These files are:
- coordinates file ($.pdb$)
- structure file ($.psf$)
- force field parameter file

- configuration file

When a molecule is inserted the coordinates file is created. To created the structure file we use the *Tools* menu of the GUI. Figure 9 shows the menu.
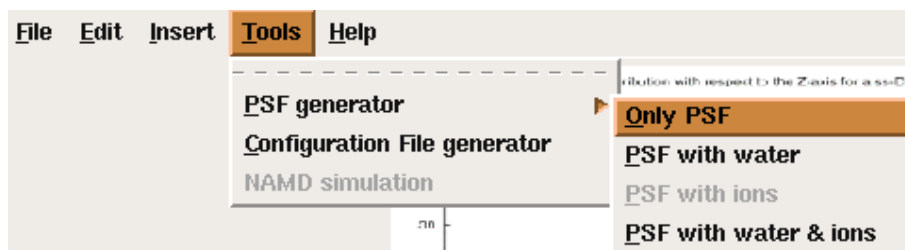

Figure 9. Menu to create the structure file.

To save the coordinates and structure files we used the *Save PDB* and *Save PSF* options of the *File* menu.

The force field parameter file was edited manually to create the spacial forces of our polymers and fiber.

To create the configuration file we have a window with some simulation parameters, for the others we used the default ones. Figure 10 shows the window that create the configuration file.
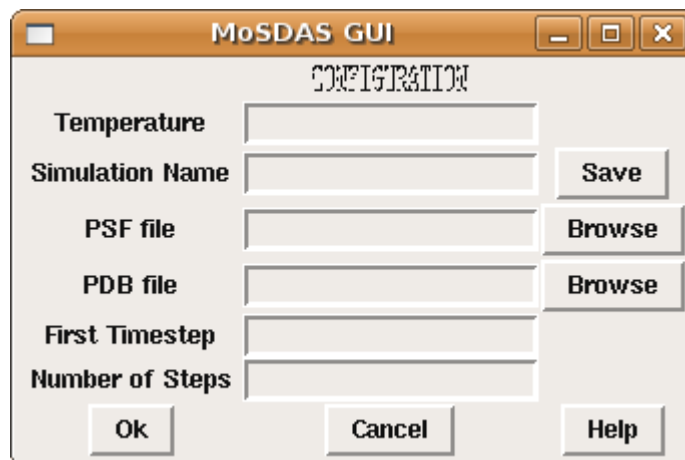

Figure 10. Windows to create the configuration file.

4.3 Phase 3 and 4

These phases are currently in construction.

All these windows and the software in general are working, and they have been used to try to run MD simulation manually. This GUI is good tool for people who want to study the hybrid systems.

5. Conclusions

This GUI greatly simplified the setup of the simulation and avoids the most of the errors in the setup process. The time of setup and make all the necessary file to run a NAMD simulation was reduced from hours to minutes. The GUI are going to be a good tool to perform MD simulation of CNT-Polymer hybrids.

6. Future work

To complete the phases 3 and 4 of the GUI.

7. Acknowledgments

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