A graphical user interface to molecular dynamics simulation software for the study of CNT-Polymer hybrids

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Objectives

To develop tools with:

- easy to use interface,
- physical simulation parameters for this type of simulation,
- distribution functions suited for this study.

Importance

Application to:

- functionalized nanotubes in sensor's fabrication,
- study of the effects of the interactions between CNT and biological polymers for biomedial research.

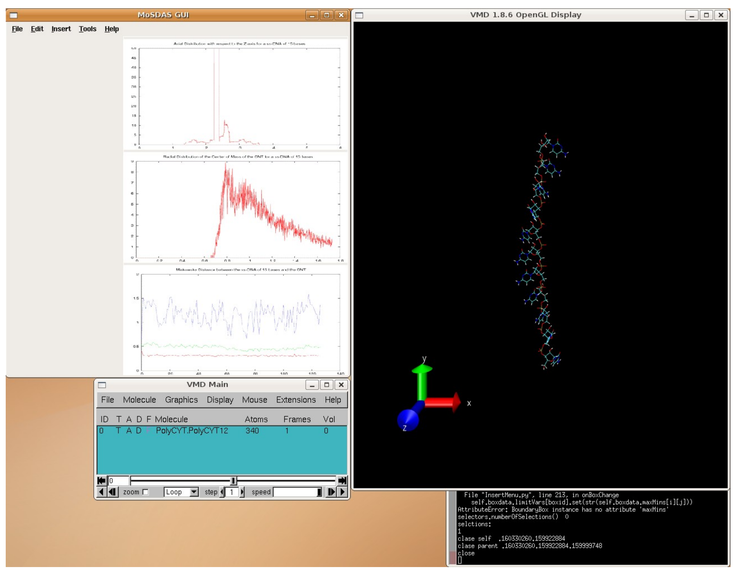
Molecular Dynamics & MoSDAS

- *Molecular Dynamics simulation* are the study of the atoms by computer simulations.
- *MoSDAS* is the Model building, Simulation and Data Analysis Script (Python Module).

MoDAS GUI

Has four phases:

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



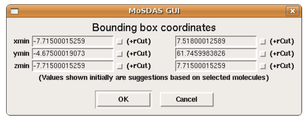
Phase 1

- To insert polymers and/or fiber we use the next widows.

- Other stuffs:
  - the Selection window

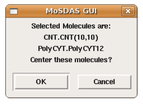
after you select a molecule...

  - insert a Box for the selected molecule

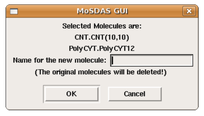


  - move the selected molecule

  - center the selected molecule



  - if you have more than one molecule inserted you can do a merge to have only one molecule



Phase 3

- This phase is currently in construction.

Phase 4

- **Graphical Visualization of ππ-Stacking of Polymer Rings over CNTs**
  - Program that finds ππ-stacking and shows them on screen utilizing *wxPython* and *.pdb* files
- We are going to incorporate all the metrics to MoSDAS GUI after we complete the Phase 3.

Phase 2

- To run a NAMD simulation we need:
  - coordinates file (*.pdb*)
  - structure file (*.psf*)
  - force field parameter file
  - configuration fie
- When a molecule is inserted MoSDAS create a *.pdb* file for this molecule.
- To create the *.psf* file we use the Tools menu of MoSDAS GUI.

- To save the *.pdb* and *psf* file

- The force field parameter is edited manually to create the special forces of our polymers and fiber.
- To create the configuration file we have a window with some simulation parameters, for the other parameters we use the default ones.

Conclusions

- MoSDAS 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.
- MoSDAS GUI are going to be a good tool to perform MD simulation of CNT-Polymer hybrids.

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