Improving Usability of Molecular Dynamics Simulation Software

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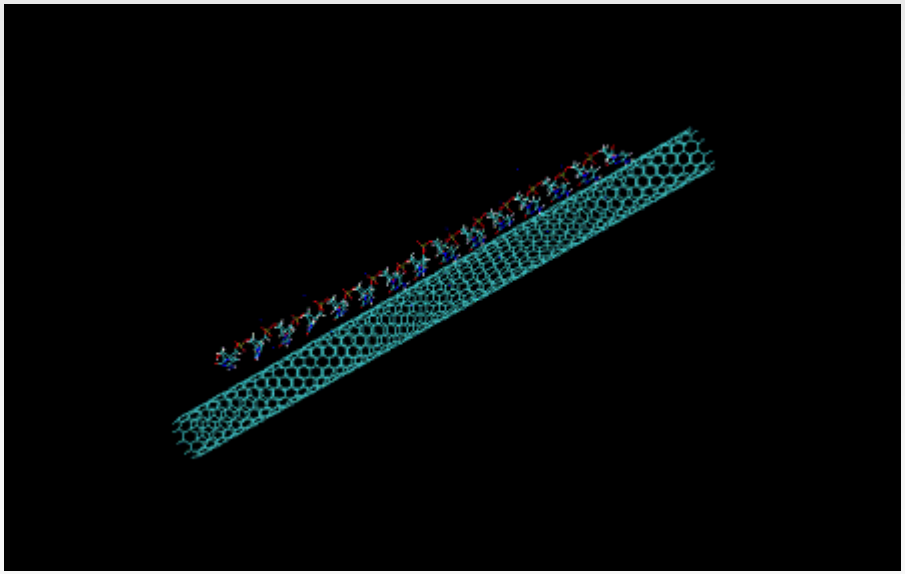
Molecular Dynamics Simulations

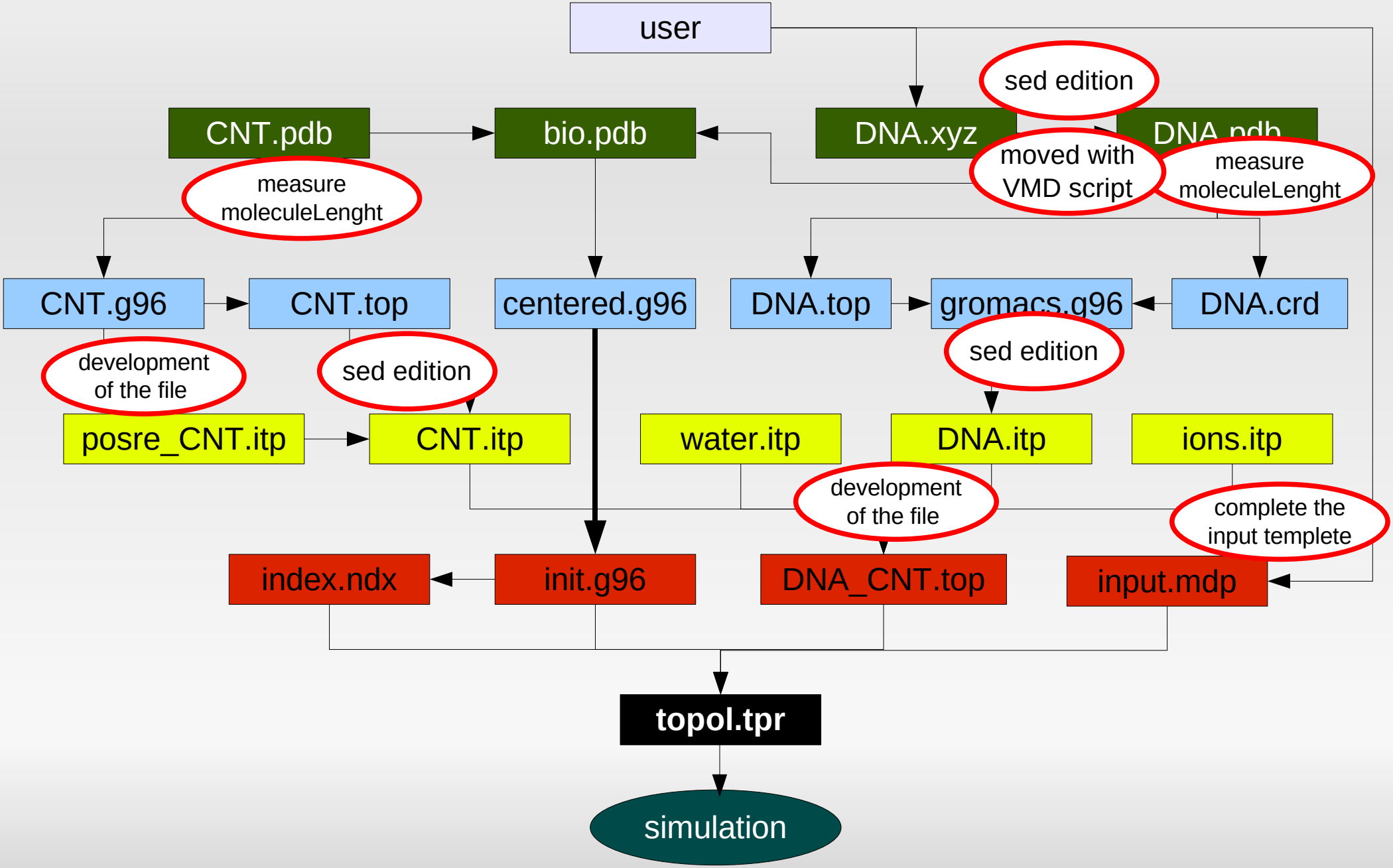
- Molecular Dynamics simulation are the study of the atoms by computer simulations.



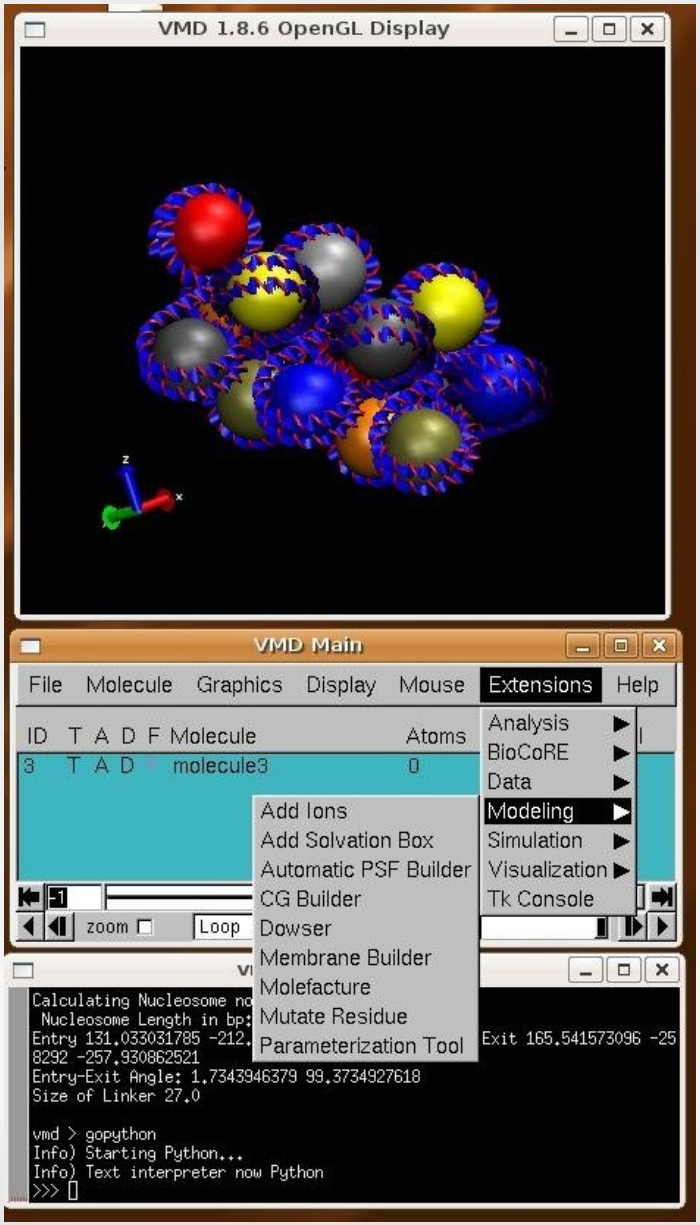
Available MD Software

- **GROMACS**
  - editconf
  - x2top
  - make_ndx
  - gen_box
- **Tinker**
  - nucleic
  - xyzpdb
- **NAMD**
  - VMD
  - psfgen
  - solvate
  - minmax
- **Amber**
  - xleap
  - tleap

Requirements to setup a simulation

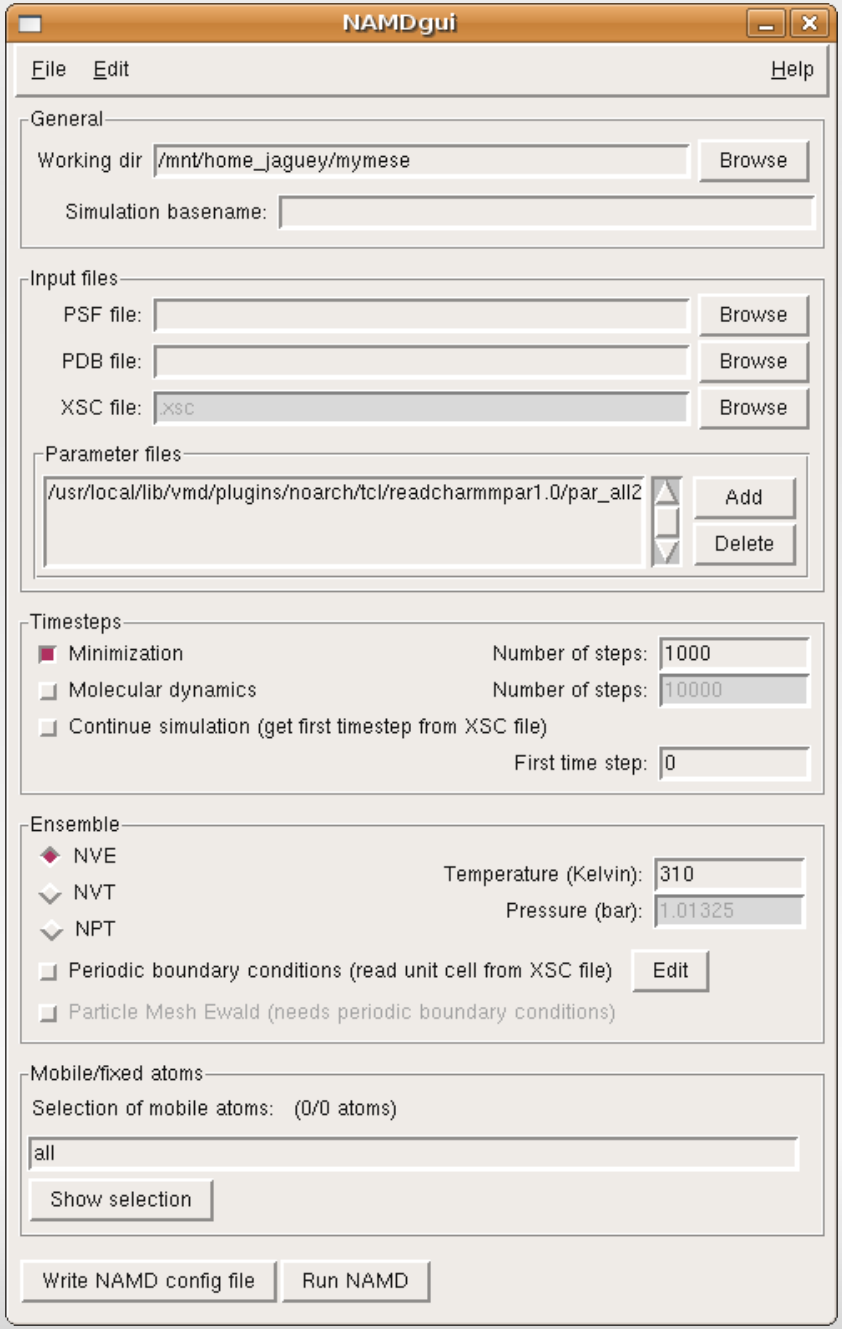


Visual Molecular Dynamics (VMD)



- Main purpose is molecule visualization
- Additional functionality added as extensions
- Built-in Python language interpreter with:
  - Tkinter
  - library for interacting with VMD features

VMD Extensions Usability Problems



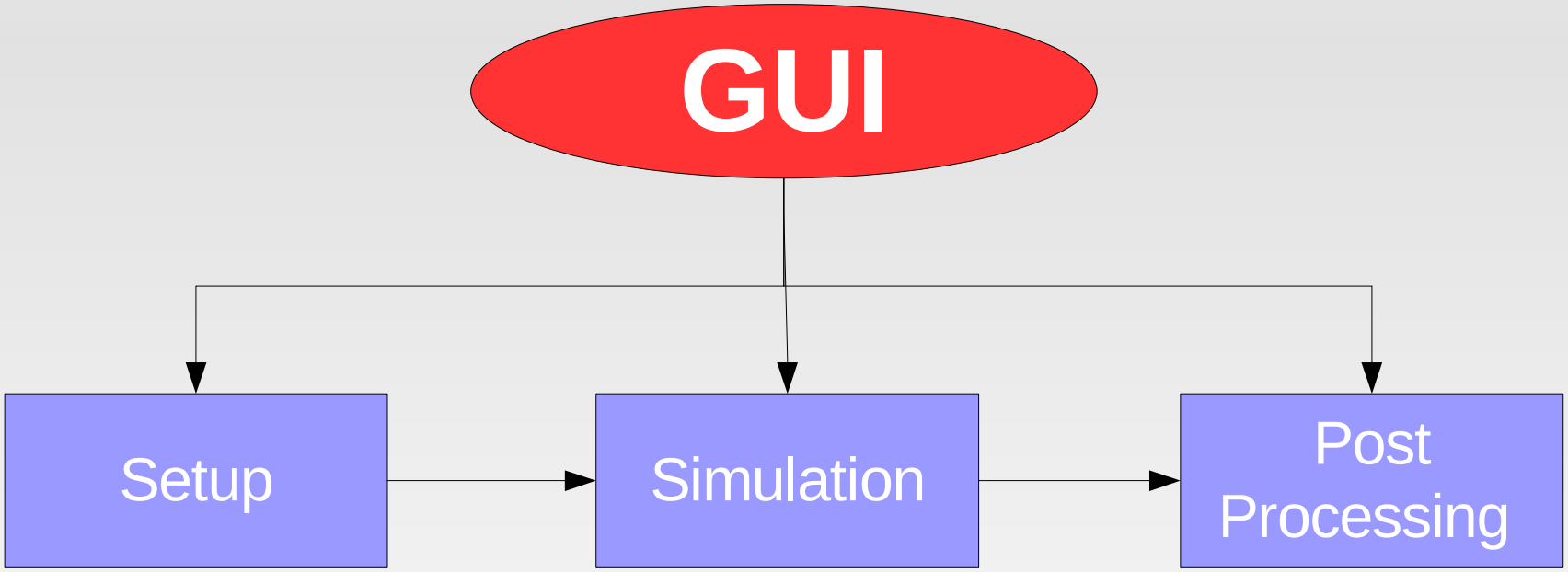
Problem

To develop a Molecular Dynamics Simulation software for Fiber-Polymer Hybrid systems that avoids the actual problems of usability.

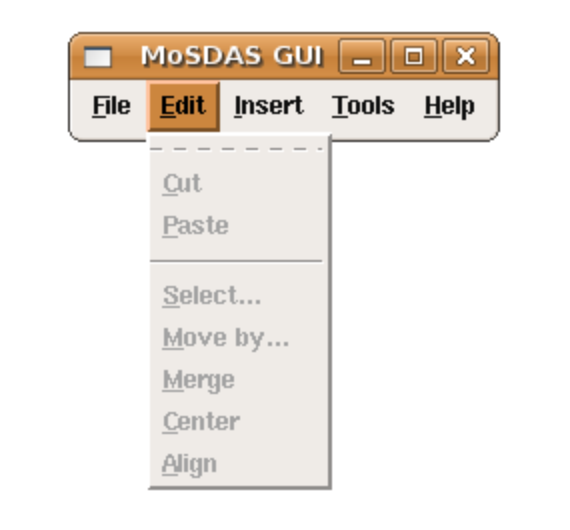
MoSDAS and VMD

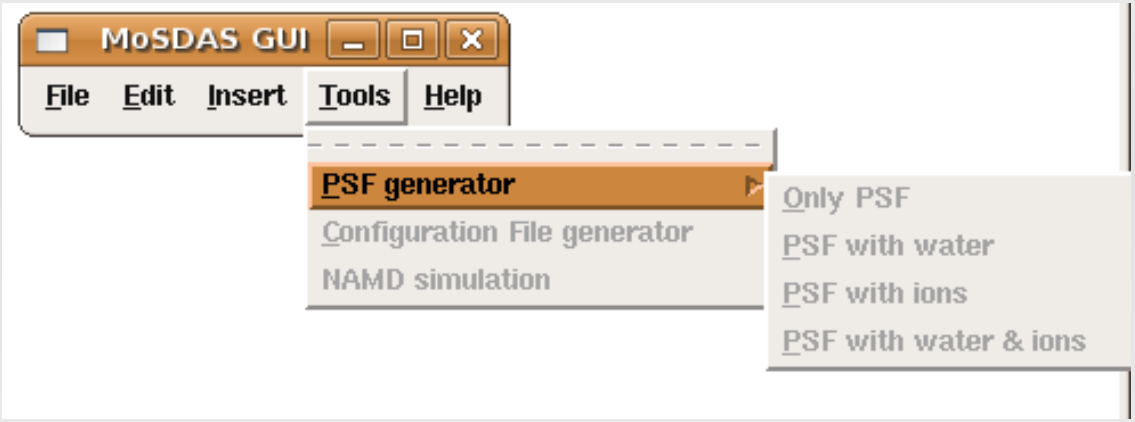
- VMD Python Library
- MoSDAS Library
  - by Computational Science Group of UPR-H

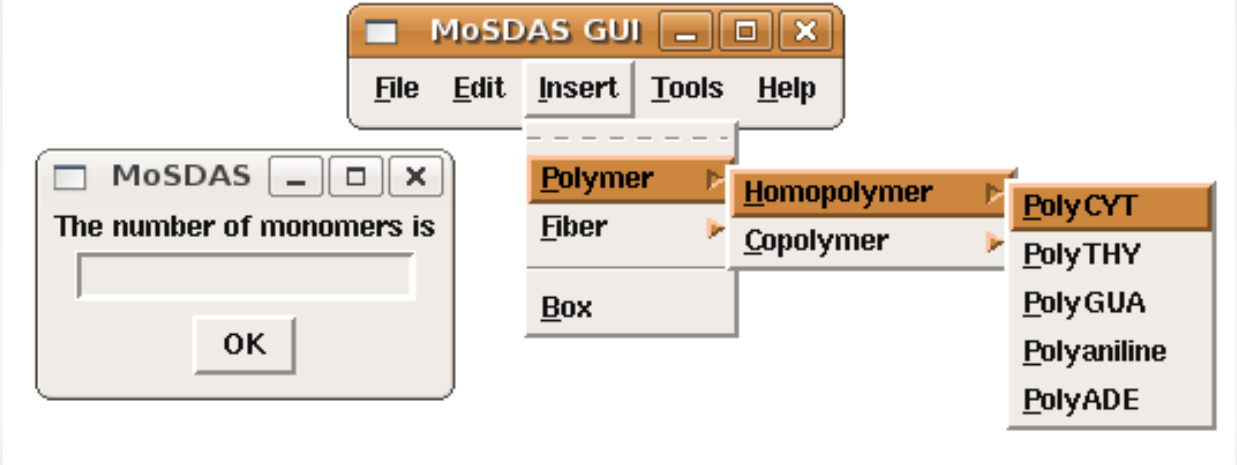
MoSDAS GUI



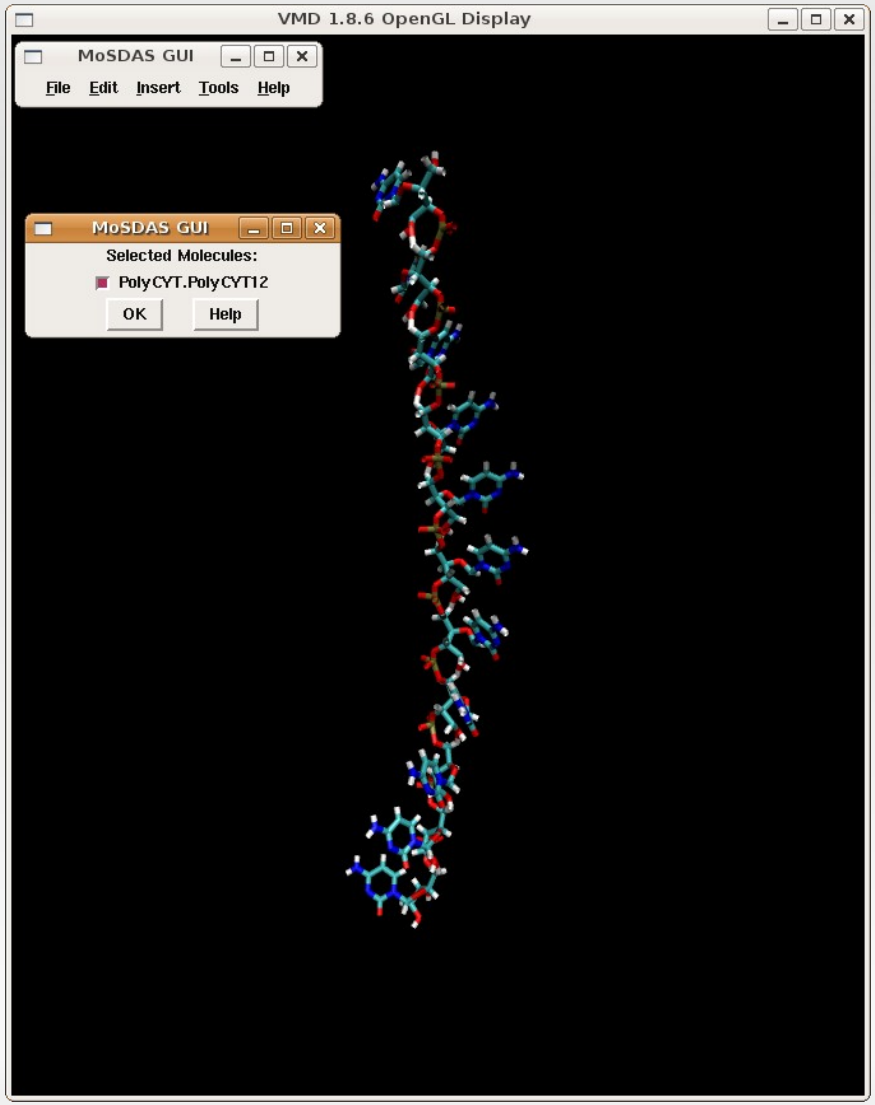
MoSDAS GUI

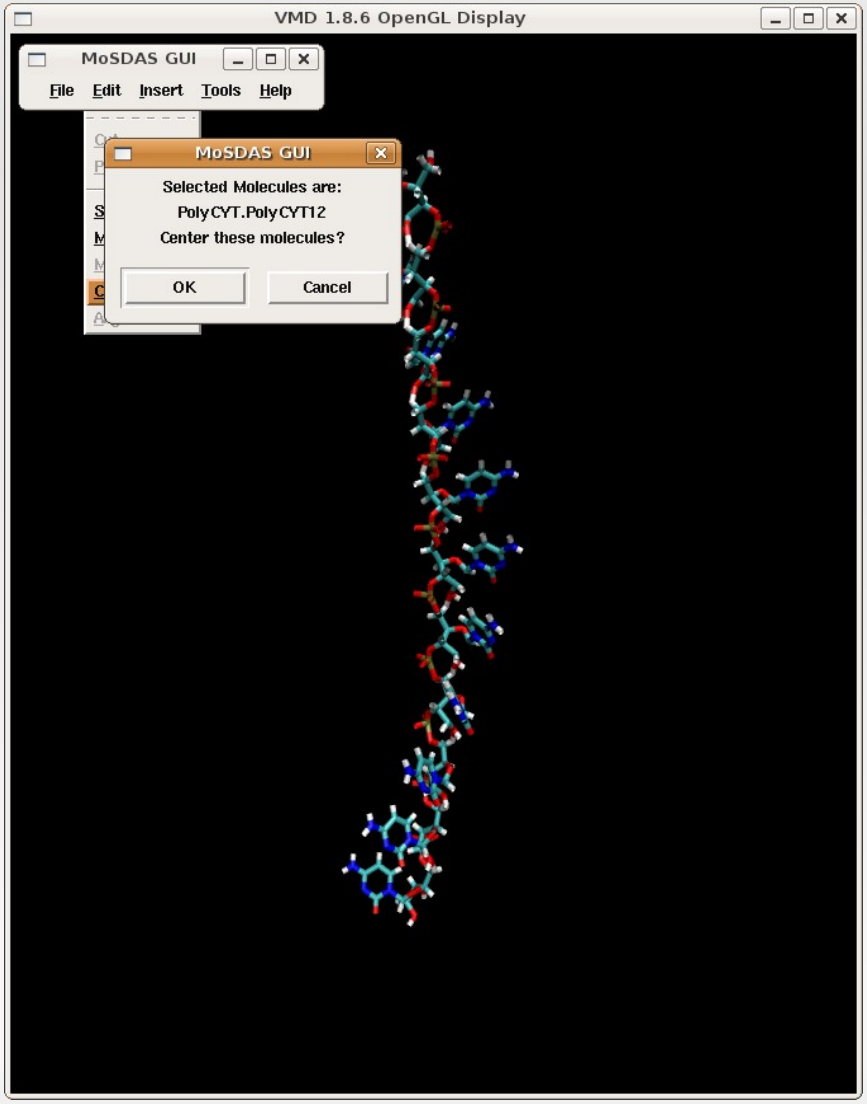

MoSDAS GUI
File
Edit
Insert
Tools
Help
Cut
Paste
Select...
Move by...
Merge
Center
Align


MoSDAS GUI
File
Edit
Insert
Tools
Help
PSF generator
Configuration File generator
NAMD simulation
Only PSF
PSF with water
PSF with ions
PSF with water & ions

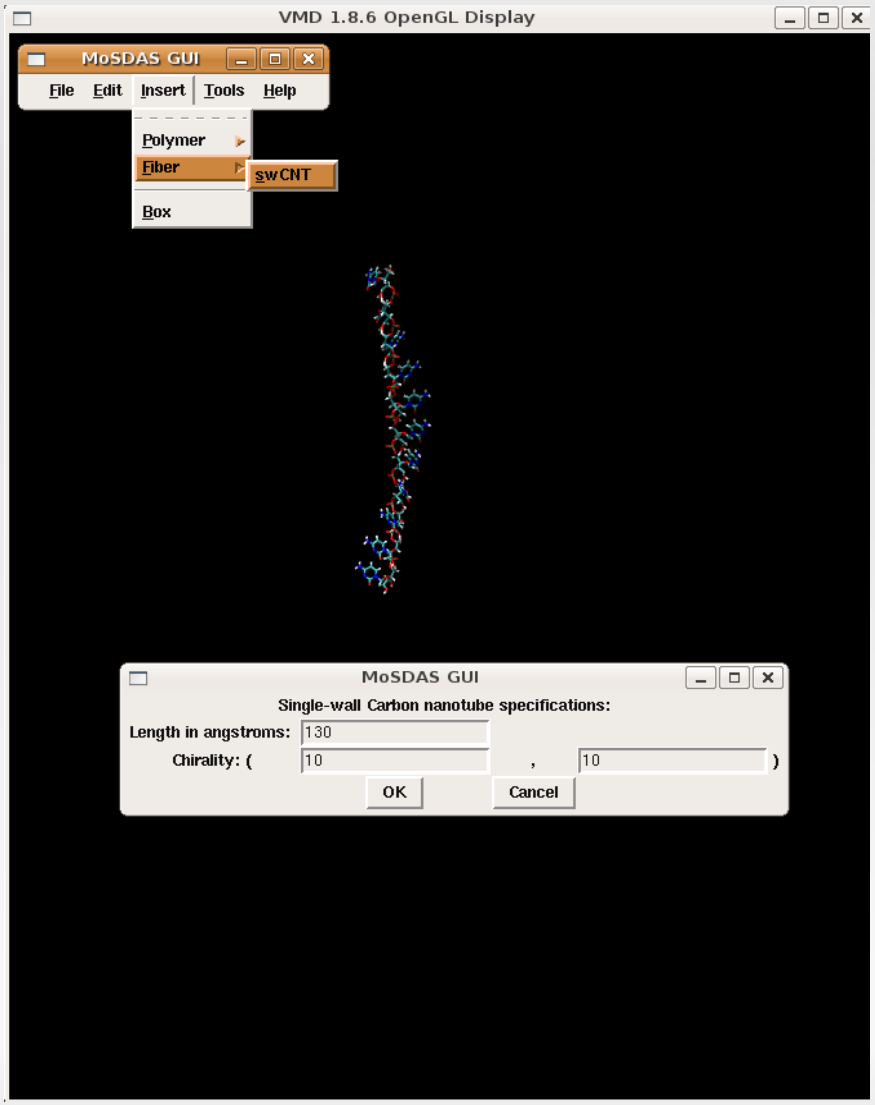

MoSDAS GUI
File
Edit
Insert
Tools
Help
MoSDAS
The number of monomers is
OK
Polymer
Fiber
Box
Homopolymer
Copolymer
PolyCYT
PolyTHY
PolyGUA
Polyaniline
PolyADE

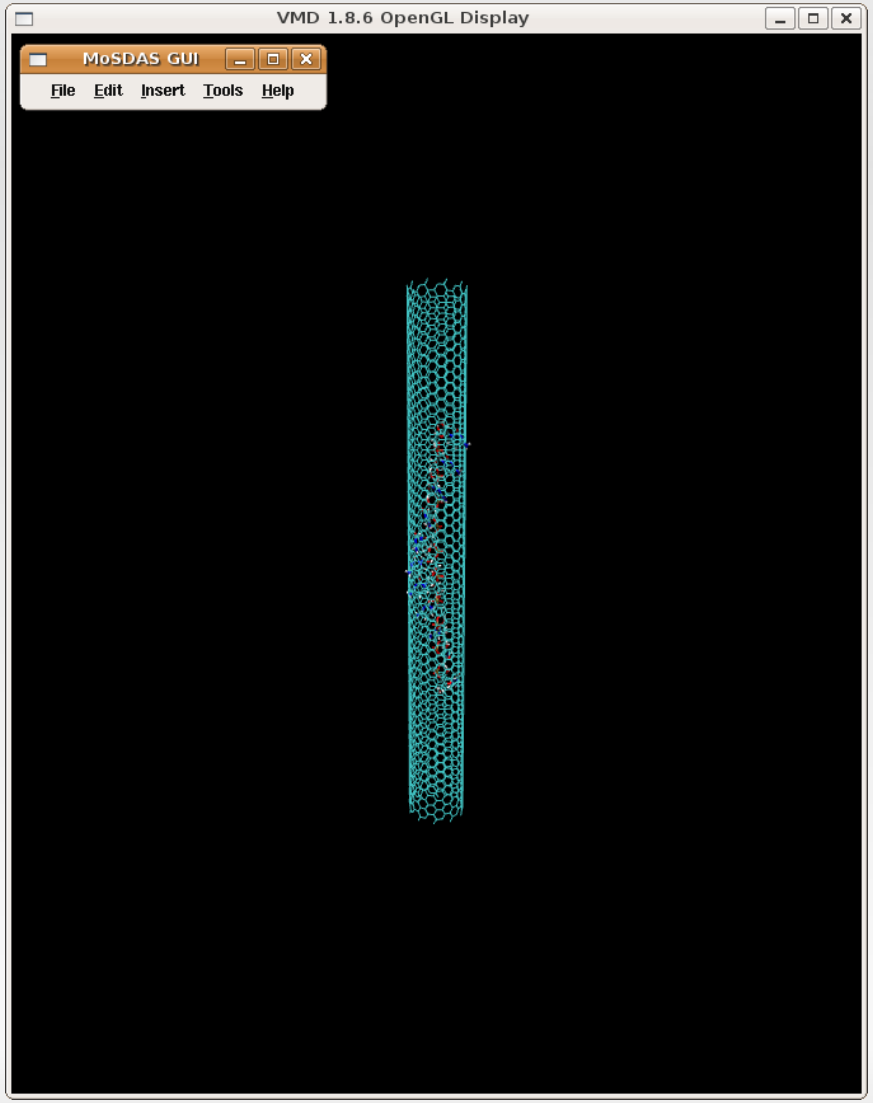
MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File Edit Insert Tools Help
MoSDAS GUI
Selected Molecules:
PolyCYT.PolyCYT12
OK
Help

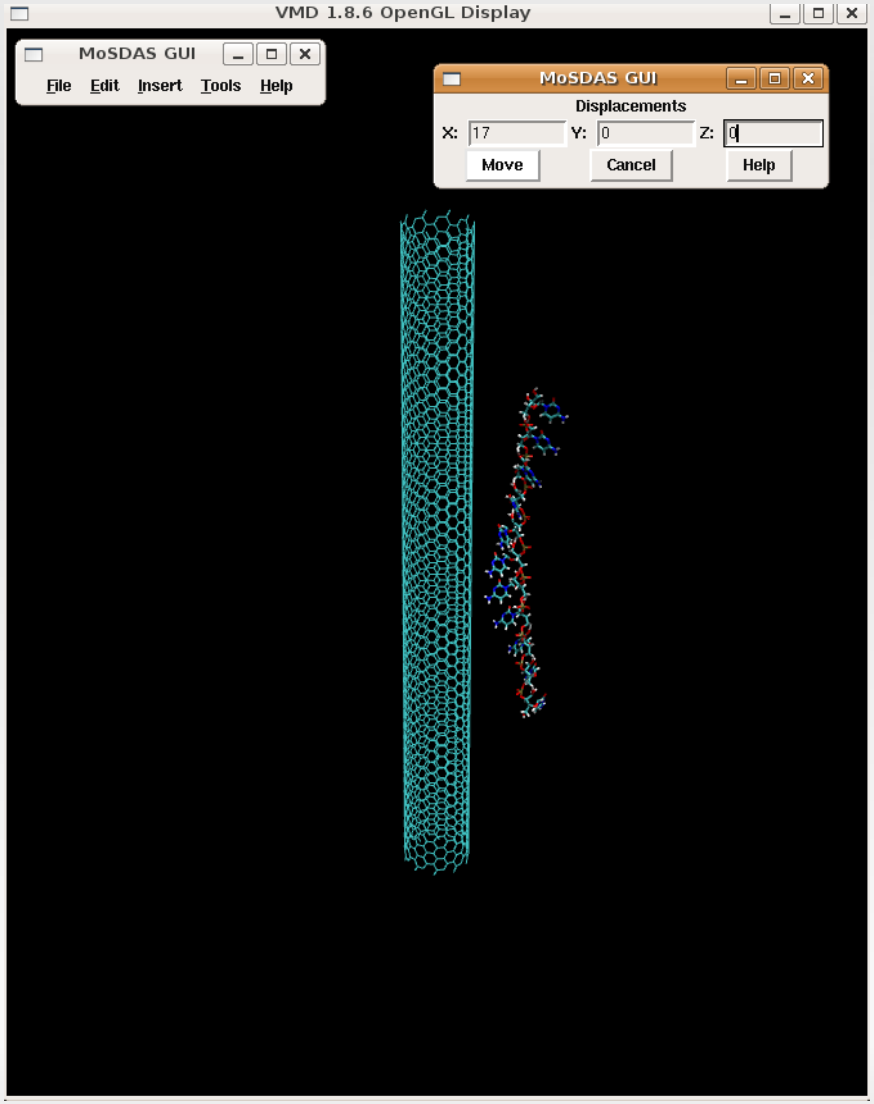

VMD 1.8.6 OpenGL Display
MoSDAS GUI
File Edit Insert Tools Help
MoSDAS GUI
Selected Molecules are:
PolyCYT.PolyCYT12
Center these molecules?
OK
Cancel

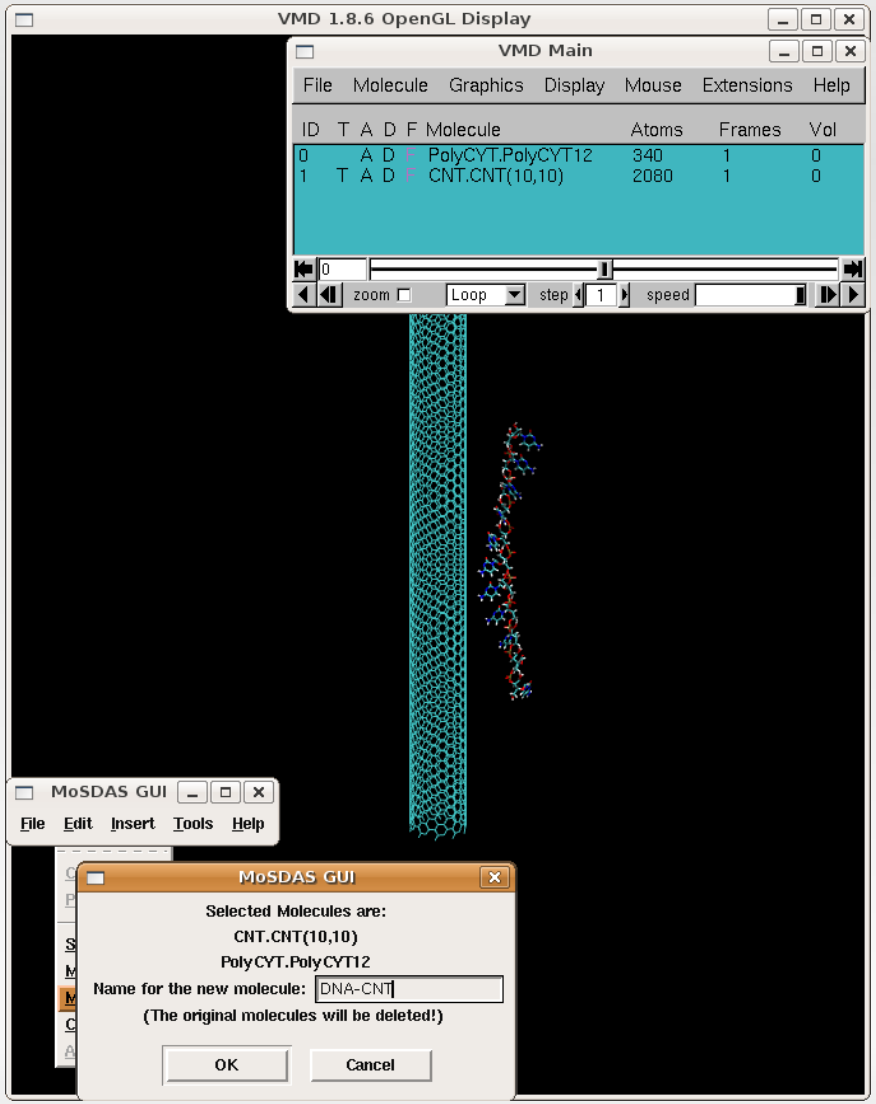
MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help
Polymer
Fiber
swCNT
Box
MoSDAS GUI
Single-wall Carbon nanotube specifications:
Length in angstroms: 130
Chirality: (10 , 10)
OK
Cancel

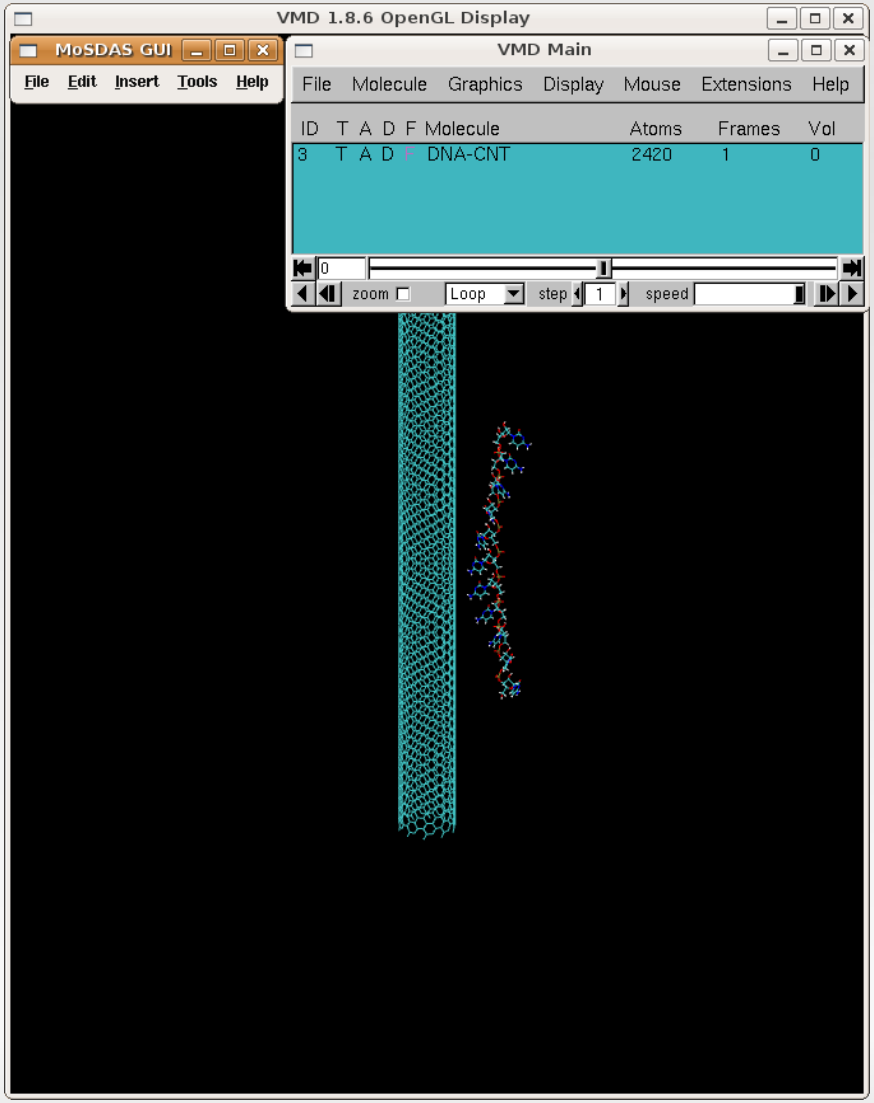

VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help

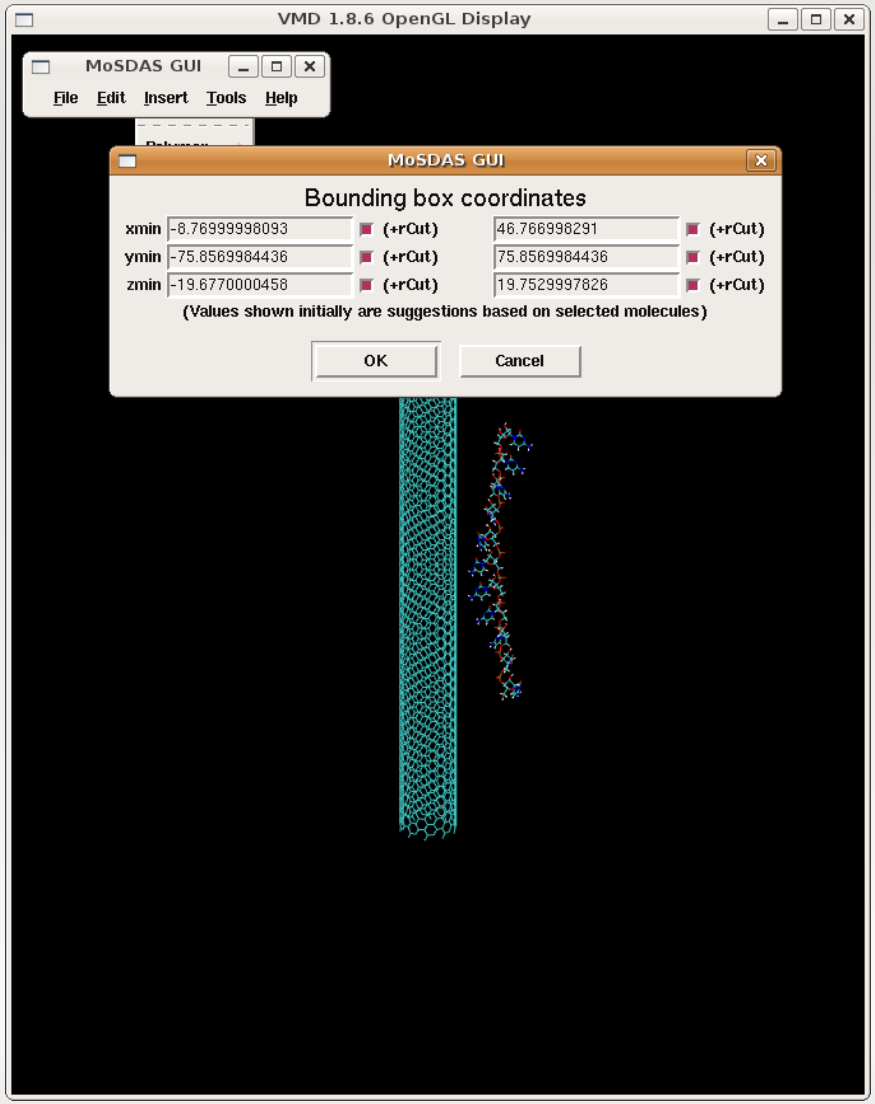
MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File Edit Insert Tools Help
MoSDAS GUI
Displacements
X: 17 Y: 0 Z: 0
Move Cancel Help

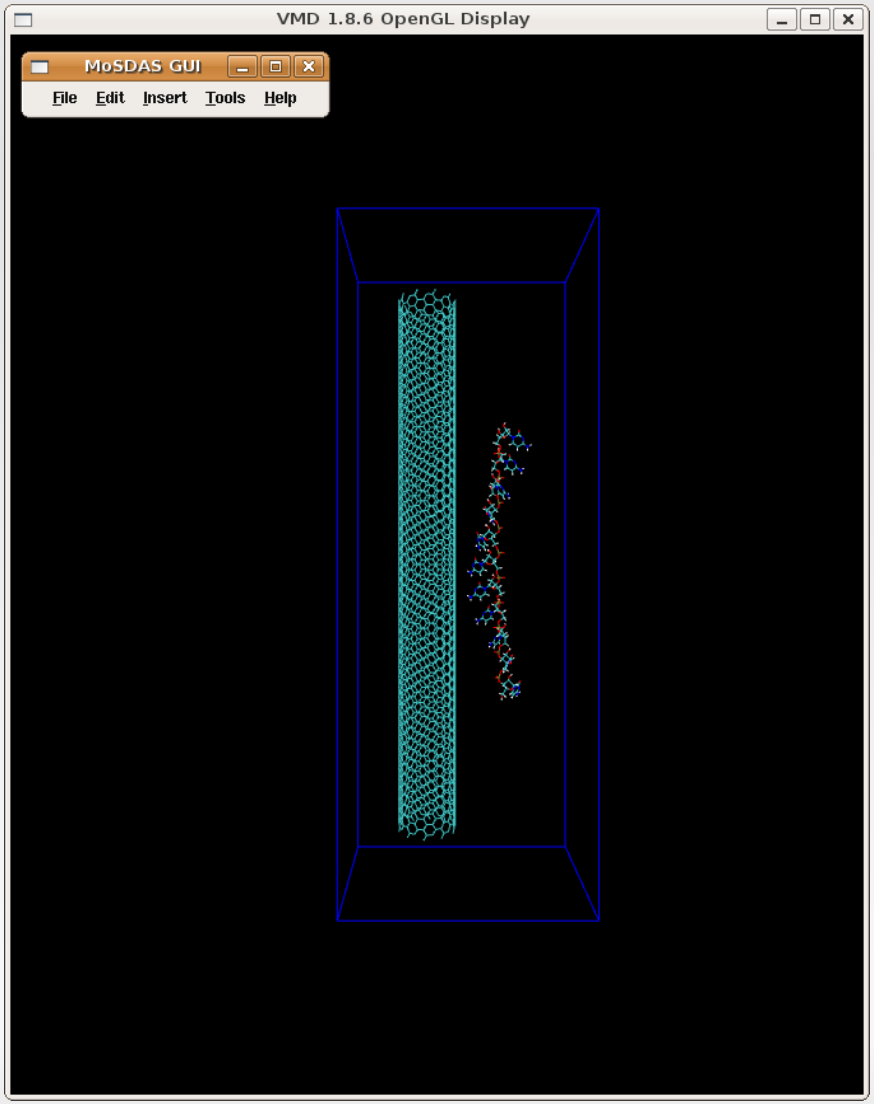

VMD 1.8.6 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F PolyCYT.PolyCYT12 340 1 0
1 T A D F CNT.CNT(10,10) 2080 1 0
zoom Loop step 1 speed
MoSDAS GUI
File Edit Insert Tools Help
MoSDAS GUI
Selected Molecules are:
CNT.CNT(10,10)
PolyCYT.PolyCYT12
Name for the new molecule: DNA-CNT
(The original molecules will be deleted!)
OK Cancel

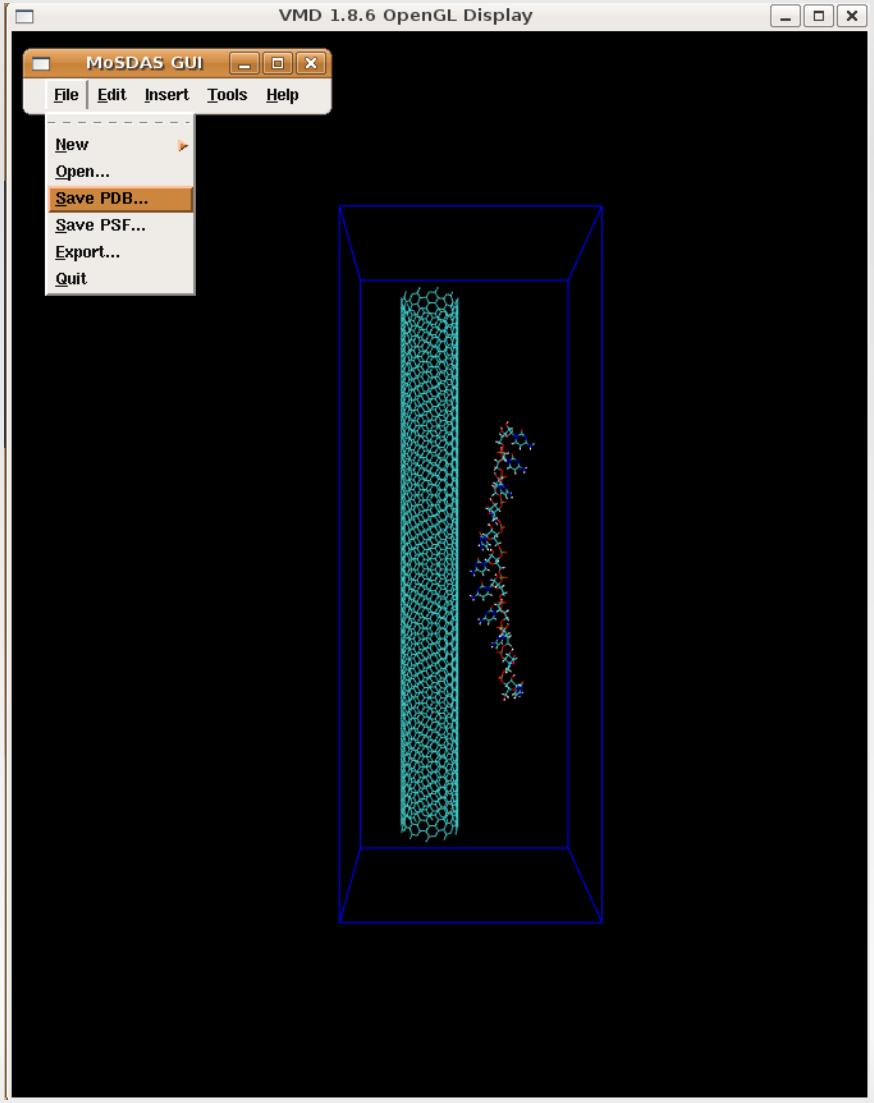
MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File Edit Insert Tools Help
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
3 T A D F DNA-CNT 2420 1 0
zoom
Loop
step
1
speed

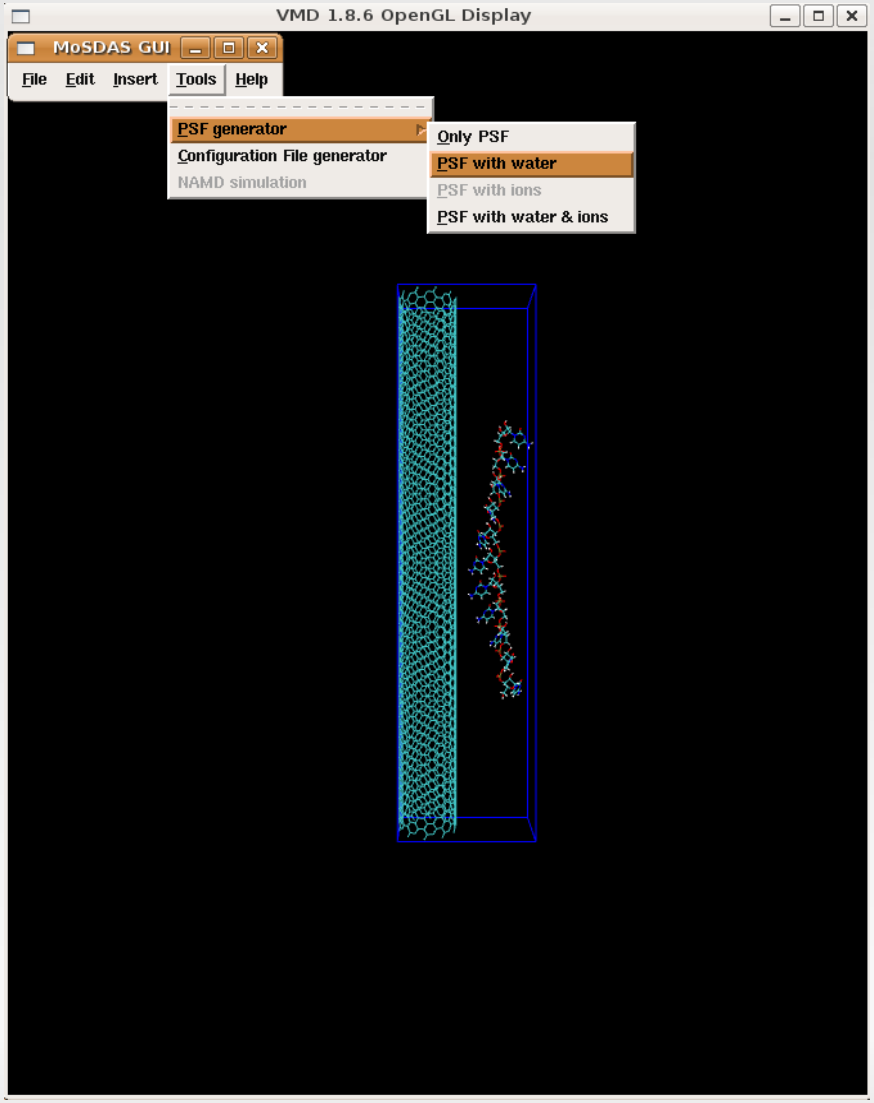

VMD 1.8.6 OpenGL Display
MoSDAS GUI
File Edit Insert Tools Help
MoSDAS GUI
Bounding box coordinates
xmin -8.76999998093 (+rCut) 46.766998291 (+rCut)
ymin -75.8569984436 (+rCut) 75.8569984436 (+rCut)
zmin -19.6770000458 (+rCut) 19.7529997826 (+rCut)
(Values shown initially are suggestions based on selected molecules)
OK
Cancel

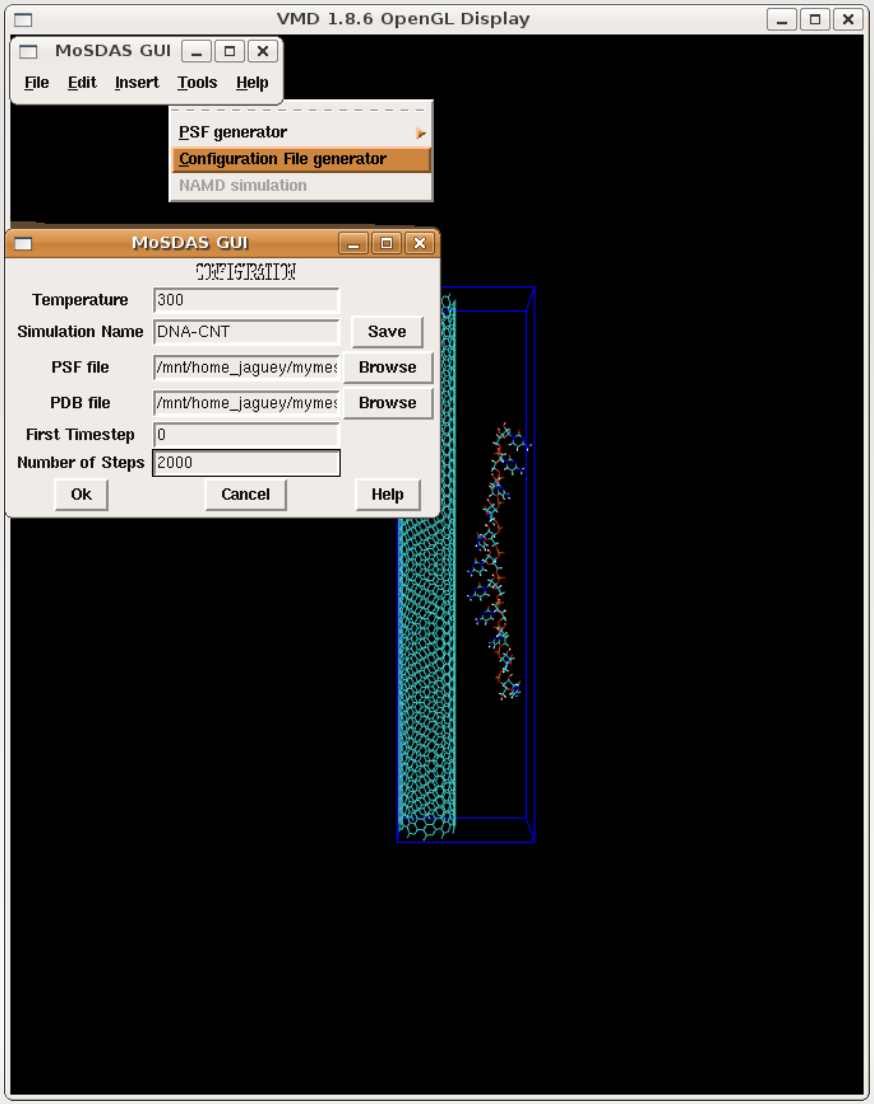
MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help
New
Open...
Save PDB...
Save PSF...
Export...
Quit

MoSDAS GUI


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help
PSF generator
Configuration File generator
NAMD simulation
Only PSF
PSF with water
PSF with ions
PSF with water & ions


VMD 1.8.6 OpenGL Display
MoSDAS GUI
File
Edit
Insert
Tools
Help
PSF generator
Configuration File generator
NAMD simulation
MoSDAS GUI
CONFIGRATION
Temperature
300
Simulation Name
DNA-CNT
Save
PSF file
/mnt/home_jaguey/mymes
Browse
PDB file
/mnt/home_jaguey/mymes
Browse
First Timestep
0
Number of Steps
2000
Ok
Cancel
Help

MoSDAS GUI Video

Conclusions

- MoSDAS GUI greatly simplifies the setup of the simulation and aviods the risk of errors in the setup process.
- The time to setup and make all the necesary files to run a MD simulation was reduced from hours to minutes.
- MoSDAS GUI are going to be a good tool to perform MD simulations of CNT-Polymer hybrids.

Acknowledgments

- UPR-Humacao MARC Program
- PREM (NSF-DMR-353730)
- URMAA (NSA-H98230-04-C-0486)

References

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- *Cristian C. and Johnson A., ”DNA-Decorated Carbon Nanotubes for Chemical Sensing*”, Nano Letters, Vol. 5, No. 9, 2005, 1774-1778.
- Visual Molecular Dynamics, http://www.ks.uiuc.edu/Research/vmd/