Conformation of ss-DNA around sw-CNTs

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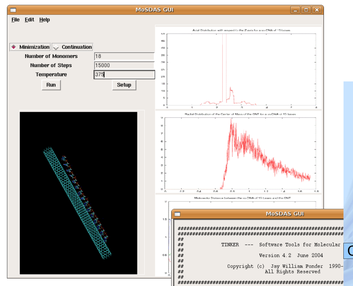
URMAA

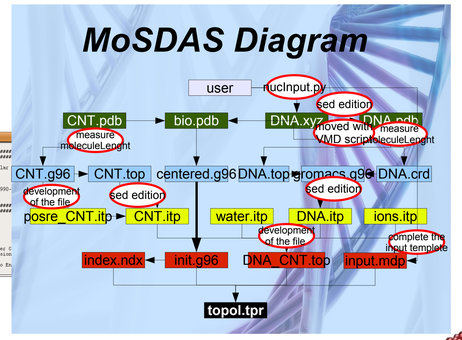
Objectives

To develop tools with:
- easy to use interface,
- integration of complex scripts for classical MD simulations,
- physical simulation parameters for these type of simulation,
- distribution functions suited for this study.

Importance

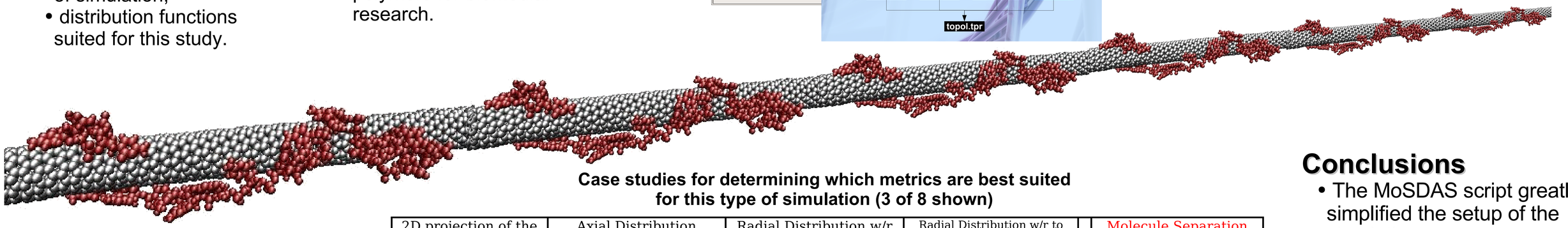
Application to:
- functionalized nanotubes in sensors' fabrication,
- study of the ffects of the interactions between CNT and biological polymers for biomedial research.





MoSDAS-GUI

- Integrates four classical MD simulation packages using four programing languages.
- Incorporate two metrics designed specially for study the conformation of DNA-CNT hybrids.



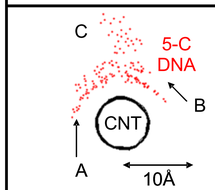
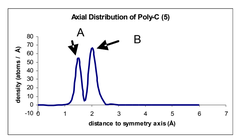
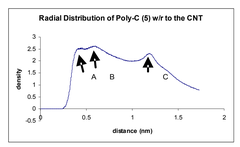
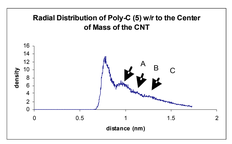
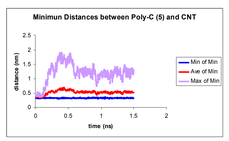
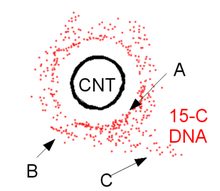
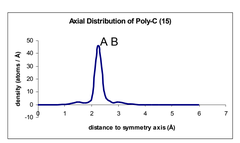
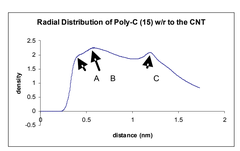
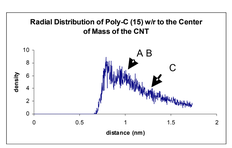
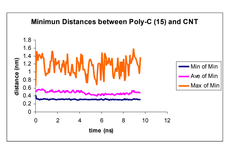
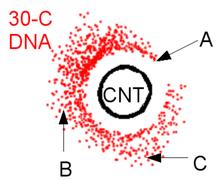
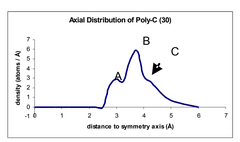
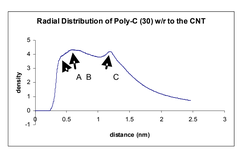
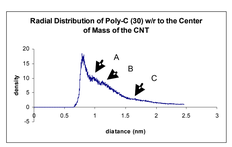
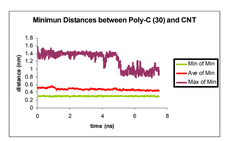
Distribution Functions

- (2) Radial distribution
  - ➔ w/r to CNT and w/r to the center of mass
  - ➔ both are from GROMACS (*g_rdf)*
- Axial distribution
  - ➔ based on an expanding cylinder centered in the symmetry axis of the CNT

Other Function

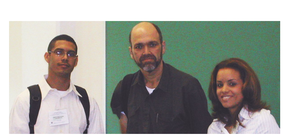
- Molecule separation distances
  - ➔ based on the maximum, minimum and average distance of the Poly-C atoms and the CNT

Case studies for determining which metrics are best suited for this type of simulation (3 of 8 shown)

2D projection of the system	Axial Distribution	Radial Distribution w/r to the CNT	Radial Distribution w/r to the center of Mass of the CNT	Molecule Separation Distances
				
				
				

Conclusions

- The MoSDAS script greatly simplified the setup of the simulation.
- Molecule separation distance graphs provide good time-dependent information about how well the ss-DNA is conforming around the CNT.
- The axial distribution function was best suited as an indicator of how the DNA atoms conform around the CNT.
- Radial distribution w/r to the CNT could be use as a validation.



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