Metrics for the Study of DNA-CNT Hybrids

Myrna I. Merced Serrano
Adviser: Prof. José Sotero Esteva
Department of Mathematics, University of Puerto Rico at Humacao

Background

- **Molecule separation distances**
  - These distances are based on the maximum, minimum and average distance of the Poly-C atoms and the CNT.
- **Radial distribution functions in MD**
  - They are based in how many atoms of a given type can be found at the distance r away from the points in the reference sets.
- **Axial distribution function**
  - It is based on an expanding cylinder centered in the symmetry axis of the CNT

Software

- **MoSDAS**
  - The Model building, Simulation and Data Analysis Script (MoSDAS) was developed to automate the production of the complete system.
  - Integrates four classical MD simulation packages using four programing languages.

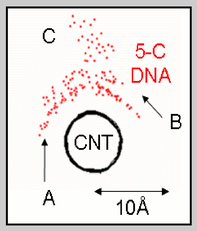
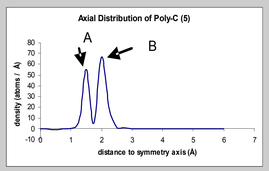
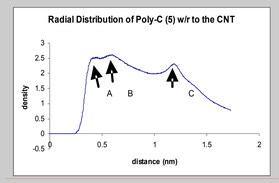
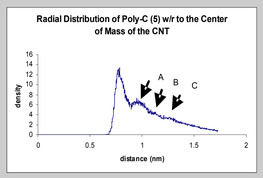
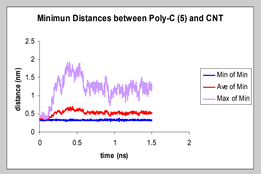
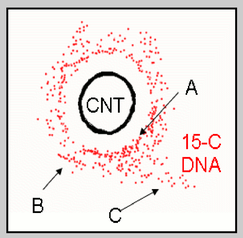
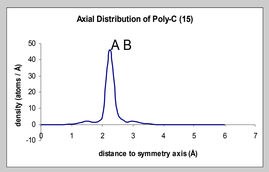
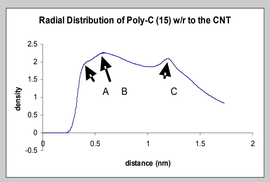
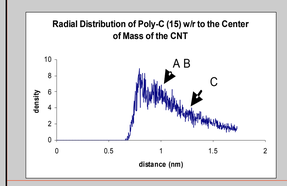
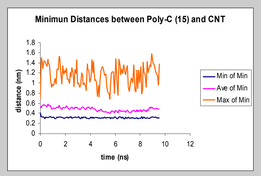
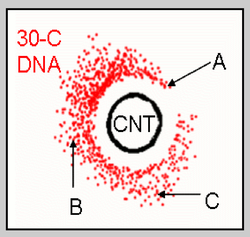
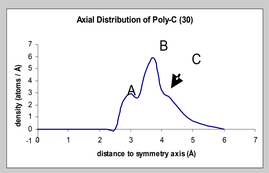
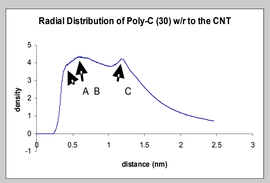
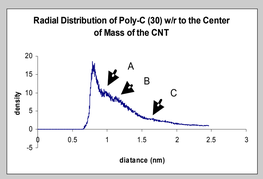
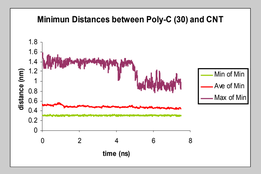
Simulations

- The obtained simulation data was of Poly-C ss-DNA of 5, 10, 15, 19, 20, 25, and 30 monomers.

Methods

- For the molecule separation a computer program was developed.
  - *Description*. The distance between an atom in the ring of the ss-DNA and all the CNT atoms was calculated. The minimum distance of each monomer was stored. Then, the minimum and maximum distances were selected and the average was calculated.
- For the calculation of the radial distribution function the program *g_rdf* that is part of the GROMACS MD package was used.
- For the calculation of the axial distribution function a computer program was developed.
  - *Description*. The distance between the coordinates (x, y) of Poly-C was measured and stored in a vector. Then the vector was sorted in an ascending position. Next the program prints out the distance and the portion of the system that have the atoms at a respective distance of the axis of symmetry. Then, the numerical derivative of each distance was calculated.
- A qualitative comparison of the developed metrics and the GROMACS metrics (radial distribution functions) was done.

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
				
				
				

Results

- Molecule separation distances between Poly-C and CNT shows how close and tight the Poly-C wraps completely around the CNT. Also, they show is the system is equilibrated or not.
- In Axial sistribution agglomerations of atoms at different levels are observed.
- Radial distributions functions don't give important information in this specific problem.

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 used as a validation.

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