MD simulations of ss-DNA conformation about CNTs: Activities Report

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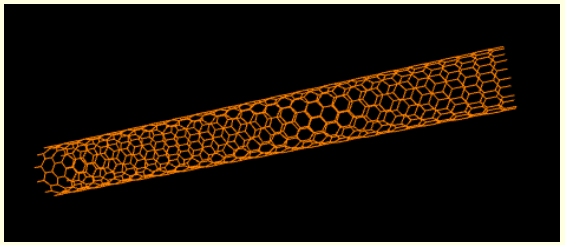
Outline

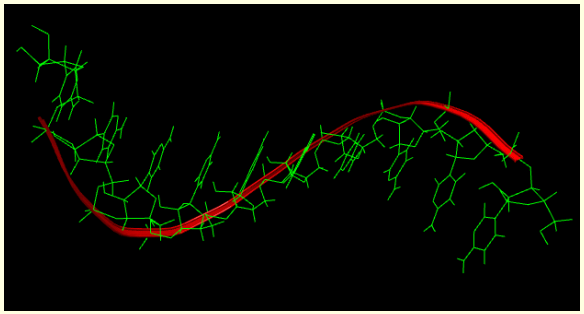
- Background
- Results presented at:
  - 3rd Annual PREM Meeting, UPRH
  - XXII SIDIM Congress, Ponce, PR
  - 27th PRISM, Carolina, PR
  - UPRH Research Day
  - 7th SSCC, Mississippi
  - NCUR-2007, California
- Current work

Background

- Molecular dynamics
  - the study of the atoms by computer simulations
- Carbon nanotubes
  - cylindrical sheets of carbon



- ss-DNA
  - DNA molecule consisting of only one chain of alternating sugars and phosphates
  - Poly-C



3rd Annual PREM Meeting

- Results:
  - Development of metrics to study how the Poly-C ss-DNA wraps into the CNT.
  - Metrics:
    - Axial Probability Distribution Function (APDF)
    - Radial Probability Function (RPF)
    - Minkowski Distance Graph (MDG)
- Conclusion:
  - The APDF and MDG gave more information for this particular simulation than the RPF.

3rd Annual PREM Meeting

COMPUTATIONAL TOOLS FOR THE STUDY OF INTERACTIONS BETWEEN ss-DNA and CNT

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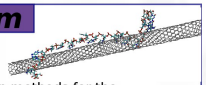
Department of Physics, University of Pennsylvania

Problem

Molecular Dynamics Simulations



Based on the interactions between a single stranded DNA (ss-DNA) and a single walled carbon nanotube (CNT).

To develop methods for the automation of the simulations of Poly-C ss-DNA of different lengths adsorbing to a CNT.

To develop metrics for the measuring of the distances between the ss-DNA and the CNT.

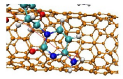
Procedure

- Development of the Model building, Simulation and Data Analysis Script (MoSDAS) to automate the production of the complete system.
- Performed molecular dynamics simulations using the GROMCS MD package.
- Development of a computer program based on the measurements of the Minkowski distance.
- Used of the radial distribution function program of the GROMACS MD package to measure the distances w/r to the CNT atoms and w/r to the center of mass of the CNT.
- Development of a computer program to measure the axial distribution of the atoms with respect to the z-axis.
- Determined which metric its the best for analyzing the data.

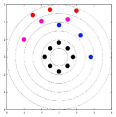
Metrics

Minkowsky Distances Graph (MDG)

Maximum, average and minimum Minkowsky distances between one atom in each of the Poly-C rings and the CNT during the simulation.



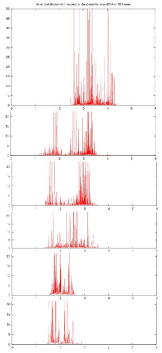
Probability Distribution Functions



Axial w/r to z-axis, Radial w/r to one atom and Radial w/r to many atoms. They are based on an expanding cylynder, an expanding sphere and many spanding spheres respectively.

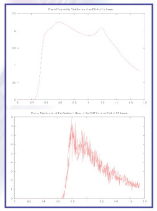
This work was supported by the *Penn-UPR Partnership for Research and Education in Materials* project (NSF-DMR-353730), the *Humacao Undergraduate Research in Mathematics to Promote Academic Achievement* program (NSA-H98230-04-C-0486), *UPRH RISE* and *National Science Foundation's Computer Science, Engineering and Mathematics Scholarships* program (NSF-0123169).

Results and Conclusions



Axial Probability Distribution Functions (APDF)

The APDFs graphs (left) show the distribution of the atoms in the ss-DNA w/r to the z-axis for ss-DNAs of 5, 10, 15, 19, 25 and 30 monomers. Agglomerations of atoms at different levels are observed for some molecules. They also show a shift to larger CNT-DNA distances as the ss-DNA length increased.

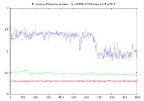


Radial Probability Functions (RPDF)

RPDFs of ss-DNA atoms w/r to the CNT atoms and w/r to the center of mass of the CNT (top right) are from (15)Poly-C. They are similar to the RPDF's of Polt-C's of length 5, 10, 19, 25 and 30 (not shown).

Minkowsky Distance Graph

MDG for (30)Poly-C (bottom right) shows when the ss-DNA wraps completely around the CNT.



Conclusions

The MoSDAS greatly simplifies and avoids errors in the simulation process. The APDF and the MDG give more significant information about this particular simulation than the RPDF's provided by the GROMACS MD package.

November 2006

XXII SIDIM Congress

- Results:
  - First prototype of MoSDAS GUI.
- Conclusions:
  - This GUI is going to be helpfully to run MoSDAS.
  - Also, it helps to avoid the errors in the process of generate the simulations.

XXII SIDIM Congress

Sistema de simulación por dinámica molecular de interacciones entre nanotubos de carbono de pared sencilla y diferentes polímeros

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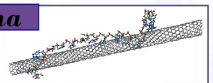
Problema

Simulaciones de Dinámica Molecular

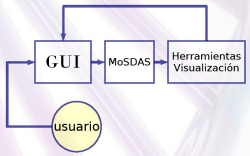


- La simulación de dinámica molecular es una técnica basada en leyes de la física que permite usar la computadora para estudiar materiales a nivel atómico.
- Los nanotubos de carbono decorados con polímeros adquieren propiedades mecánicas y eléctricas particulares.
- *Problema*: Integrar todos los métodos necesarios de la simulación de dinámica molecular entre un polímero y un nanotubo de carbono en un interfaz gráfico.

Métodos

Diseño de un prototipo de interfaz gráfico especializado para ADN:

- insumo: cantidad de monómeros, cantidad de pasos a simular y temperatura
- ejecutar el *Model building, Simulation and Data Analysis Script* (*MoSDAS*)
- mostrar el estado inicial de los átmos del sistema
- recoger los resultados
- mostrar en pantalla las gráficas de análisis

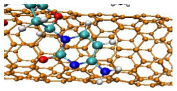


Herramientas Intergradas

Programación

Pakete Tkinter de Python
Provee:

- menú principal
- botones de selección
- campos de insumo de texto
- botones regulares
- cargar imágenes



Programas

- *MoSDAS*
- distancia entre un átomo y un conjunto de átomos
- distribución radial (*GROMACS*)
- distribución de los átomos con respecto al eje-Z
- Visual Molecular Dynamics (*VMD*) se utiliza para ver la simulación.

Medidas de análisis

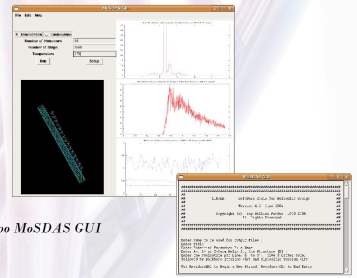
Distancia Punto-Conjunto

Calcula la distancia máxima, mínima y promedio entre un átomo de cada monómero y el nanotubo de carbono, durante la simulación.

Distribución de Probabilidad

Son dos funciones: de Eje (se utiliza el eje-Z como referencia) y Radial (con un grupo de átomos como referencia). Están basadas en un cilíndro que se expande, en el caso de la funcion de Eje y en la Radial con una esfera central que se expande junto con otras esferas.

Resultado y Conclusiones



Prototipo MoSDAS GUI

Conclusiones

El prototipo *MoSDAS GUI* es de gran ayuda para correr MoSDAS. Evita el reisgo de cometer errores. Simplifica una gran parte del trabajoy nos ayuda a tener mejor organización de los datos obtenidos.

Este trabajo fue auspiciado por el proyecto *Penn-UPR Partnership for Research and Education in Materials* (NSF-DMR-353730), el programa *Humacao Undergraduate Research in Mathematics to Promote Academic Achievement* (NSA-H98230-04-C-0486), el programa *UPRH RISE* y el programa *National Science Foundation's Computer Science, Engineering and Mathematics Scholarships* (NSF-0123169).

February 2007

27th Puerto Rico Interdisciplinary Scientific Meeting

- Results:
  - Analysis script MoSDAS
- Conclusions:
  - MoSDAS resulted in a great improvement in productivity by reducing the preparation time of the simulation from hours to seconds.
  - The development of MoSDAS simplifies and avoids the most of the errors in the simulation process.

27th Puerto Rico Interdisciplinary Scientific Meeting

A Model building, Simulation and Data Analysis Script for the Study of DNA-CNT Hybrids

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University of Puerto Rico at Humacao
Mentor: José O. Sotero Esteva

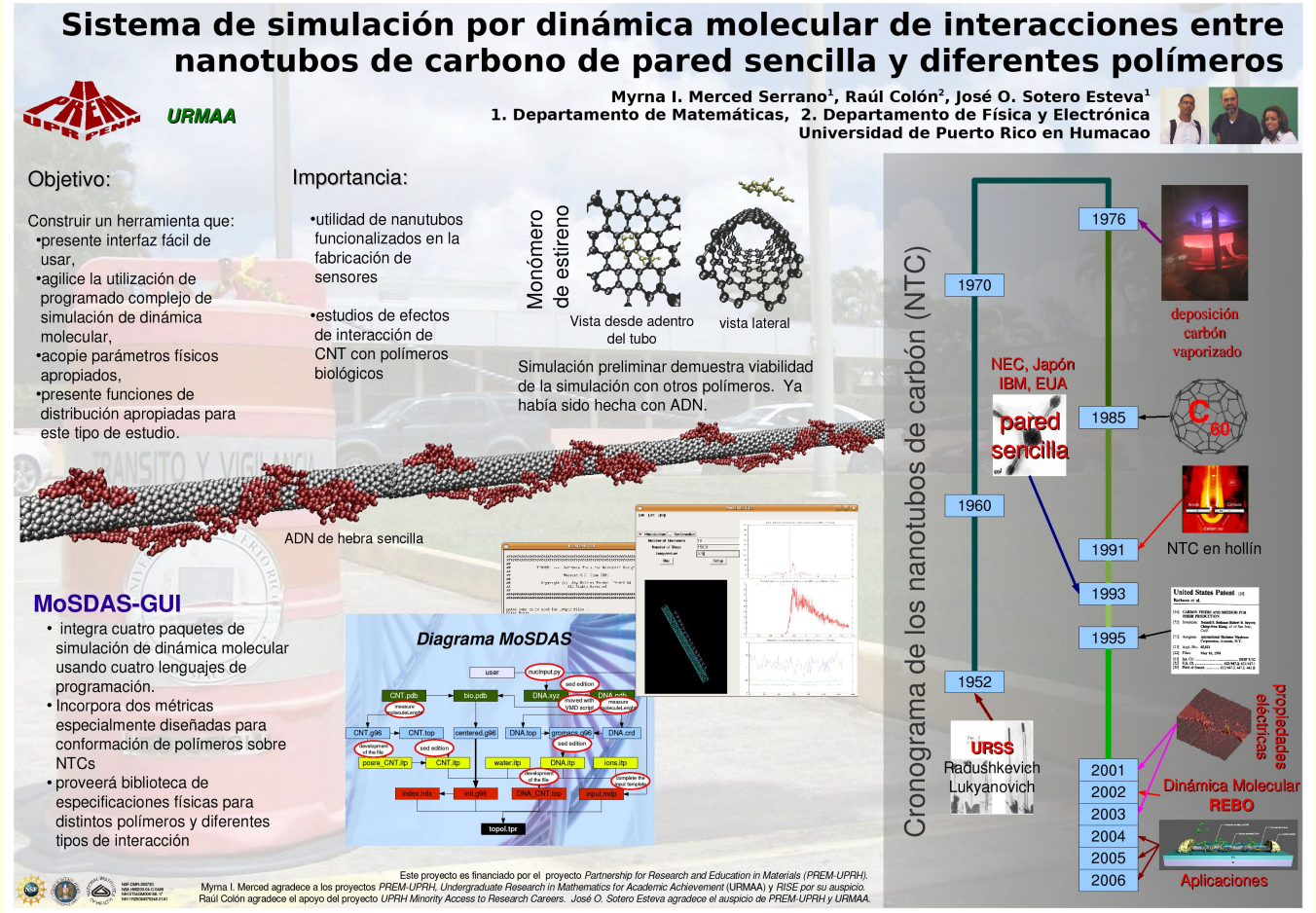
Carbon nanotubes (CNT) and single stranded DNA (ss-DNA) are both interesting and important systems in nanoscience that are completely compatible with one another. They are cylindrical sheets of carbon. CNT have diameters of approximately 1nm and lengths up to a few centimeters. Single stranded DNA (ss-DNA) is a DNA molecule consisting of only one chain of alternating sugars and phosphates. Molecular dynamics simulations are well-suited to provide insights into the fundamental properties of DNA-CNT hybrids because they enable calculation of structural properties with atomic resolution. The determination of the appropriate physical parameters for the simulations as well as the design of the process of building the simulated DNA-CNT system had been previously done. But the process was a long and labor intensive process that had to be repeated for each simulation. The Model building, Simulation and Data Analysis Script (MoSDAS) presented here was developed to automate the whole simulation process by generating the necessary parameters, calling and running all the necessary programs. All the commands of MoSDAS are in bash programming language. Some axillary programs were written in TCL and Python programming languages. The molecular dynamics simulation was done with the GROMACS MD package. MoSDAS resulted in a great improvement in productivity by reducing the preparation time of the simulation from hours to seconds. We ran eight simulations for testing purposes. The only variation in the simulations was the quantity of the ss-DNA bases. We easily produced simulations of the Poly-C ss-DNA of 5, 10, 15, 19, 20, 25, 30 and 35 bases. It was found that the development of MoSDAS simplifies and avoids the most of the errors in the simulation process.

March 2007

Research Day at UPR-Humacao

- This is an integration of Raul's work with mine.
- Is a study of Molecular dynamics simulations between CNT and different polymers.

Research Day at UPR-Humacao



March 2007

7th Southern School on Computational Chemistry and Material Science

- Results
  - Molecule separation distances show how close and tight the Poly-C wraps completely around the CNT.
  - In Axial distribution agglomerations at different levels are observed.
- Conclusions
  - Molecule separation graphs provide good time-dependent information about how well the ss-DNA is conforming about the CNT.
  - The Axial distribution function was best suited as an indicator of how the DNA atoms conforms around the CNT.

7th Southern School on Computational Chemistry and Material Science

Conformation of ss-DNA around sw-CNTs

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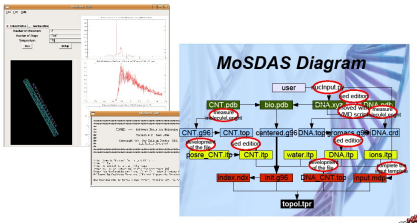
URMAA

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.

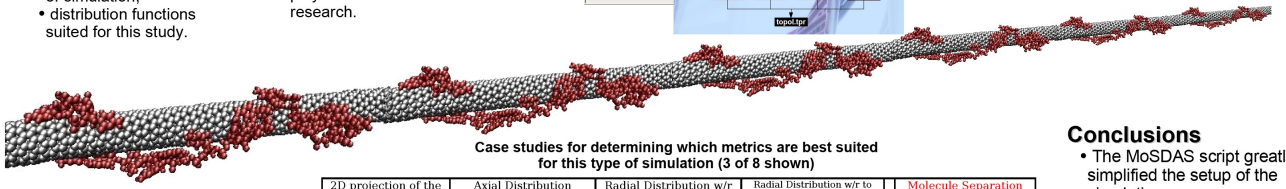
Importance

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.



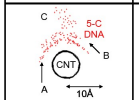
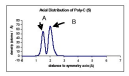
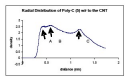
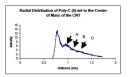
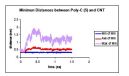
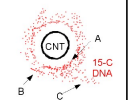
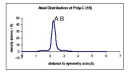
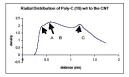
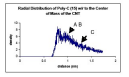
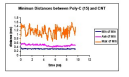
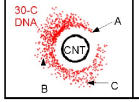
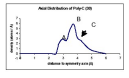
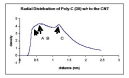
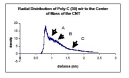
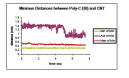
Distribution Functions

- (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.

Our in the development of this software originated from the Summer Research Experience of Myrna Merced at A.T. Johnson Laboratory under the supervision of Robert Johnson.
This work is supported by the *Penn-UPR Partnership for Research and Education in Materials* (NSF-DMR-0353730) and the *Humacao Undergraduate Research in Mathematics to Promote Academic Achievement* program (NSA-H98230-04-C-0486).

April 2007

2007 National Congress in Undergraduate Research

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

RISE URMAA

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

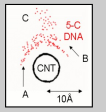
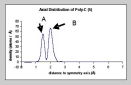
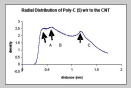
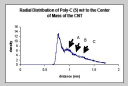
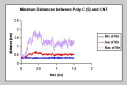
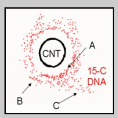
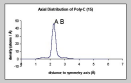
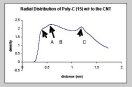
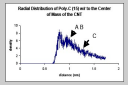
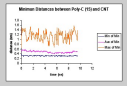
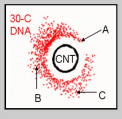
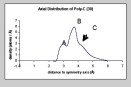
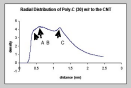
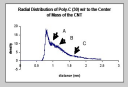
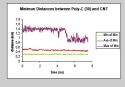
Software

- **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.

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
				
				
				

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.

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.

Our interest in the analysis of these MD simulations are originated from the Summer Research Experience of Myrna Merced at A.T. Johnson's Laboratory under the supervision of Robert Johnson.
This work is supported by the *Penn-UPR Partnership for Research and Education in Materials* (NSF-DMR-0353730), the *Humacao Undergraduate Research in Mathematics to Promote Academic Achievement* program (NSA-H98230-04-C-0486), and UPRH RISE program.

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Metrics for the Study of DNA-CNT Hybrids

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Abstract

DNA-carbon nanotube (DNA-CNT) hybrids have many useful properties important in the field of nanoscience. Molecular dynamics (MD) simulations are well-suited to provide insights into the fundamental properties of DNA-CNT hybrids because they enable calculation of structural properties with atomic resolution. Radial distribution functions are often used to detect structural properties of liquids and crystalline materials in MD simulations. In this work other metrics for measuring how well ss-DNA conforms onto CNT were defined, tested, and compared to radial distribution functions. Three measures were defined as the maximum, minimum and average of the molecule separation distances intended to measure how close and tight the ss-DNA wraps around the CNT. An axial distribution function with respect to the z-axis was also defined. It is based on an expanding cylinder centered in the symmetry axis of the CNT instead. A simple ss-DNA (Poly-C) was used for testing purposes. A complex process of model building, simulation and data analysis was completely automated as a script (MoSDAS). Simulations were performed for Poly-C's with varying number of bases. Both of the metrics defined above as well as two radial distribution functions provided by the GROMACS MD package were compared. It was found that MoSDAS greatly simplifies the simulation process and avoids errors. Also, the molecule separation based metrics provides better information than the other measures on when the ss-DNA wraps around the CNT. The axial distribution function was best suited as an indicator of how the DNA atoms conform around the CNT. Analysis of this function shows, for example, a shift to larger CNT-DNA distances as the ss-DNA length increased. A two-peak distribution suggests that different parts of the Poly-C agglomerate at different levels. This information is not evident in the usual radial distribution functions.
Keywords: Molecular Dynamics, DNA-CNT hybrids, Distribution Function

1. Introduction

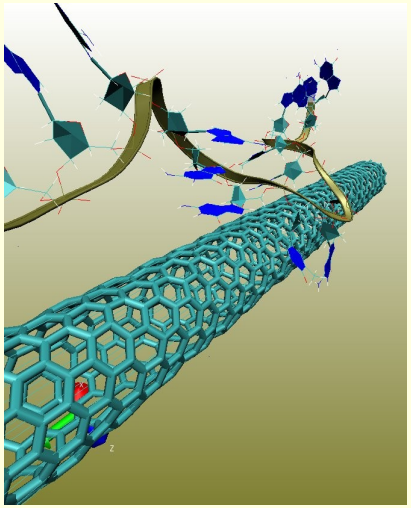
Carbon nanotubes (CNT) and single stranded DNA (ss-DNA) are both interesting and important systems in nanoscience. For example, ss-DNA-CNT hybrids have been recently used to construct nanoscale chemical sensors.[1] ss-DNA has also been used to separate and sort CNTs based on metallicity.[2] They are completely compatible with one another. Molecular dynamics (MD) simulations are well-suited to provide insights into the fundamental properties of DNA-CNT hybrids because they enable calculation of structural properties with atomic resolution.

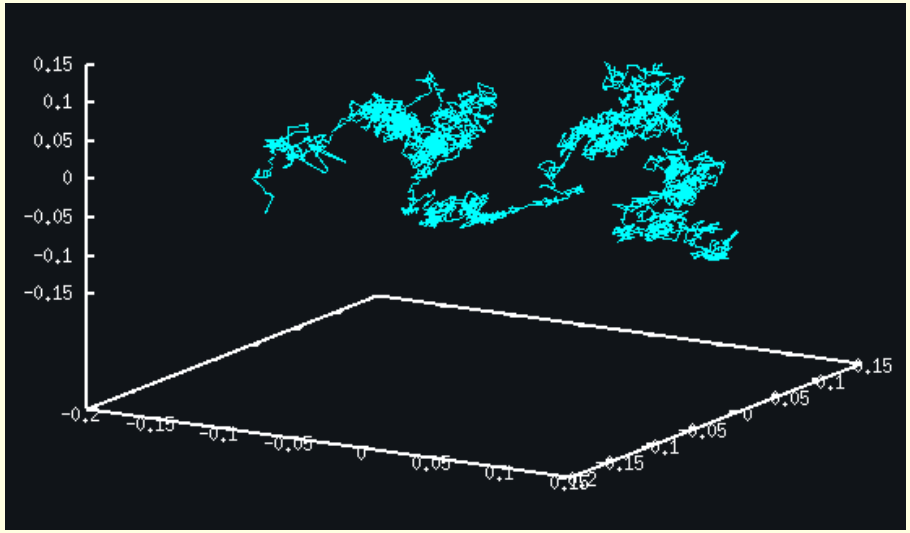
It is understood that ss-DNA attaches readily to the CNT by the $\pi - \pi$ stacking interaction.

April 2007

Current work

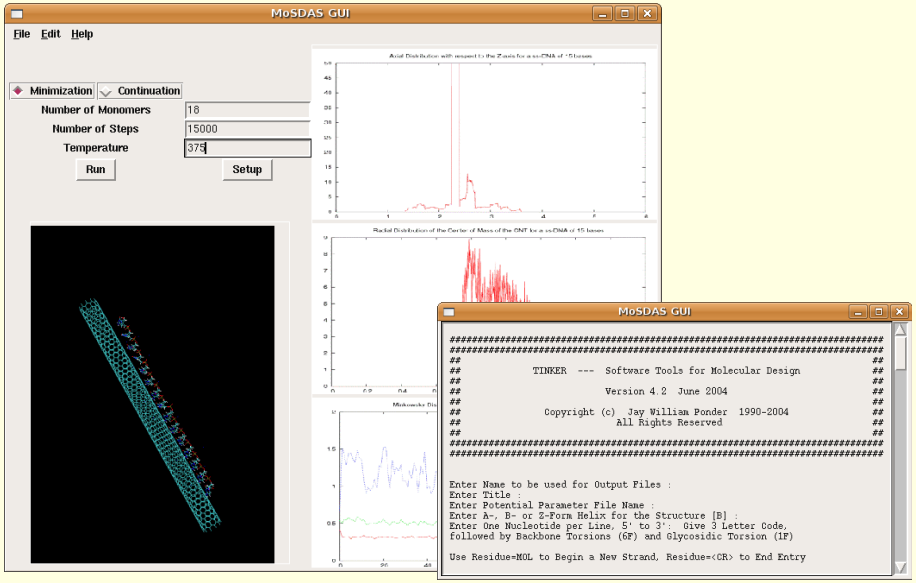
- **Principal Components Analysis in CNT-DNA conformations**
  - Frames produced by MD simulation coded as N-dimensional vector
  - PCA produces sequence of 3D (or 2D) points





Current work

- **Graphical User Interface for CNT-Polymer hybrids MD Simulations**
  - Preparation, execution and analysis of MoSDAS
  - Phython-Tkinter, independent application, VMD plug in.



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