Molecular Dynamics Simulations of ss-DNA conformation about Carbon Nanotubes

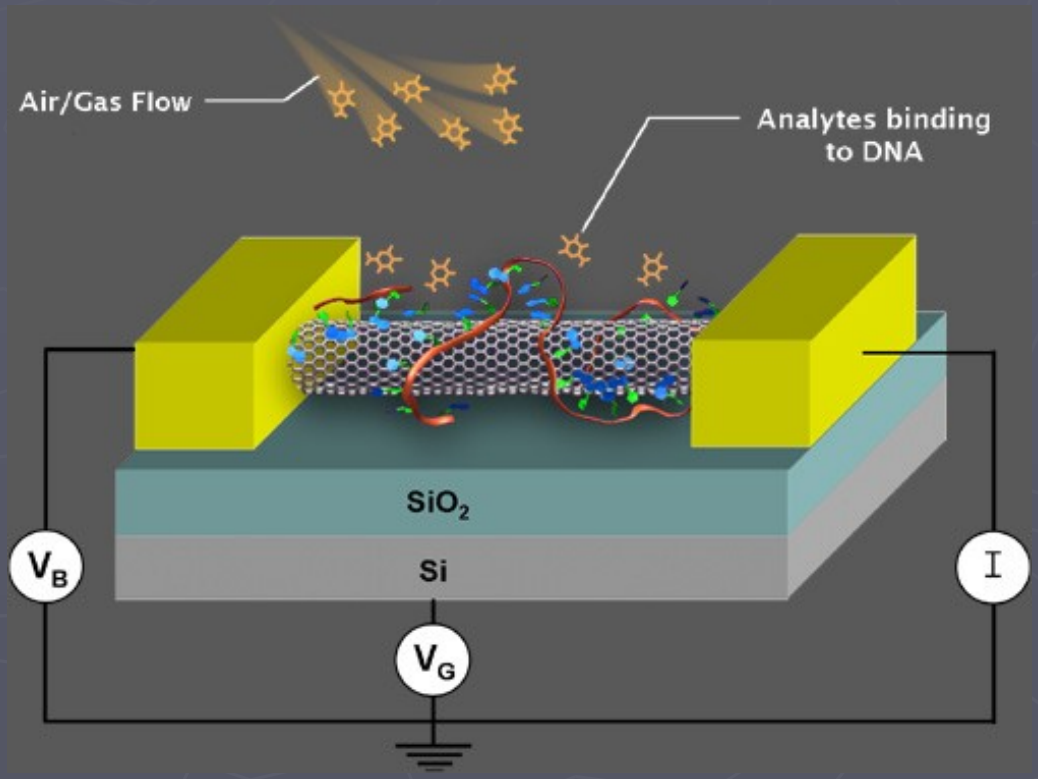
Myrna I. Merced Serrano

Computational Mathematics Program

University of Puerto Rico at Humacao

Thursday, August 31,2006

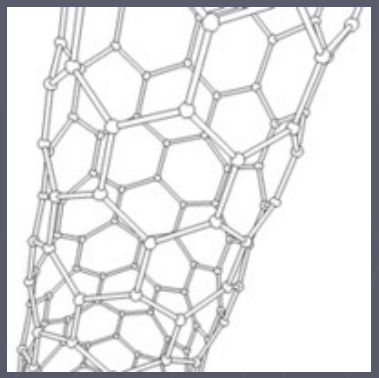
DNA-Functionalized Carbon Nanotube Chemical Sensors



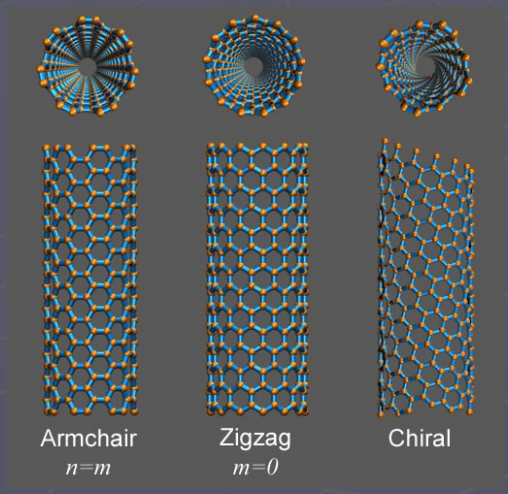
http://www.lrsm.upenn.edu/~nanophys/biosensors.html

Carbon Nanotubes

- Carbon nanotubes are cylindrical sheets of carbon that were discovered in 1991.
- Nanotubes have diameters of about 1 nm and lengths up to a few centimeters.
- Nanotubes have been a popular subject for condensed matter physics research as well as a top candidate for applications in nanotechnology.



http://en.wikipedia.org/wiki/Carbon_nanotube



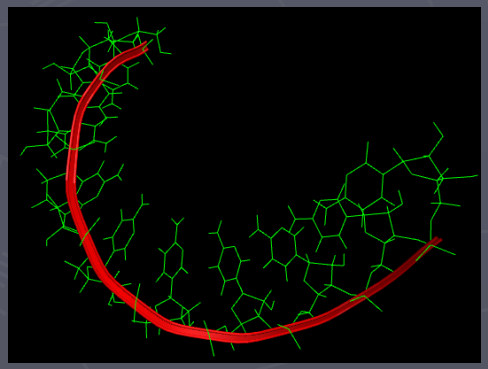
http://www.lrsm.upenn.edu/~nanophys/biosensors.html

ss-DNA and its different structures

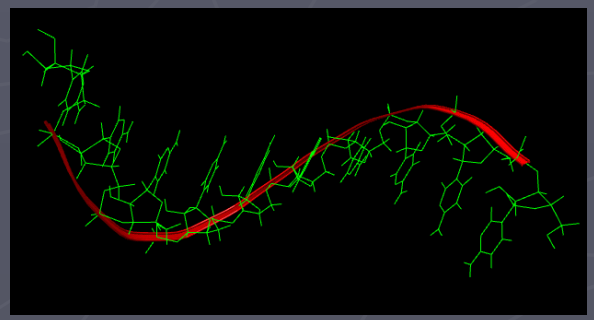
A Single-stranded DNA (ss-DNA) is a DNA molecule consisting of only one chain of alternating sugars and phosphates.

Examples:

A form →



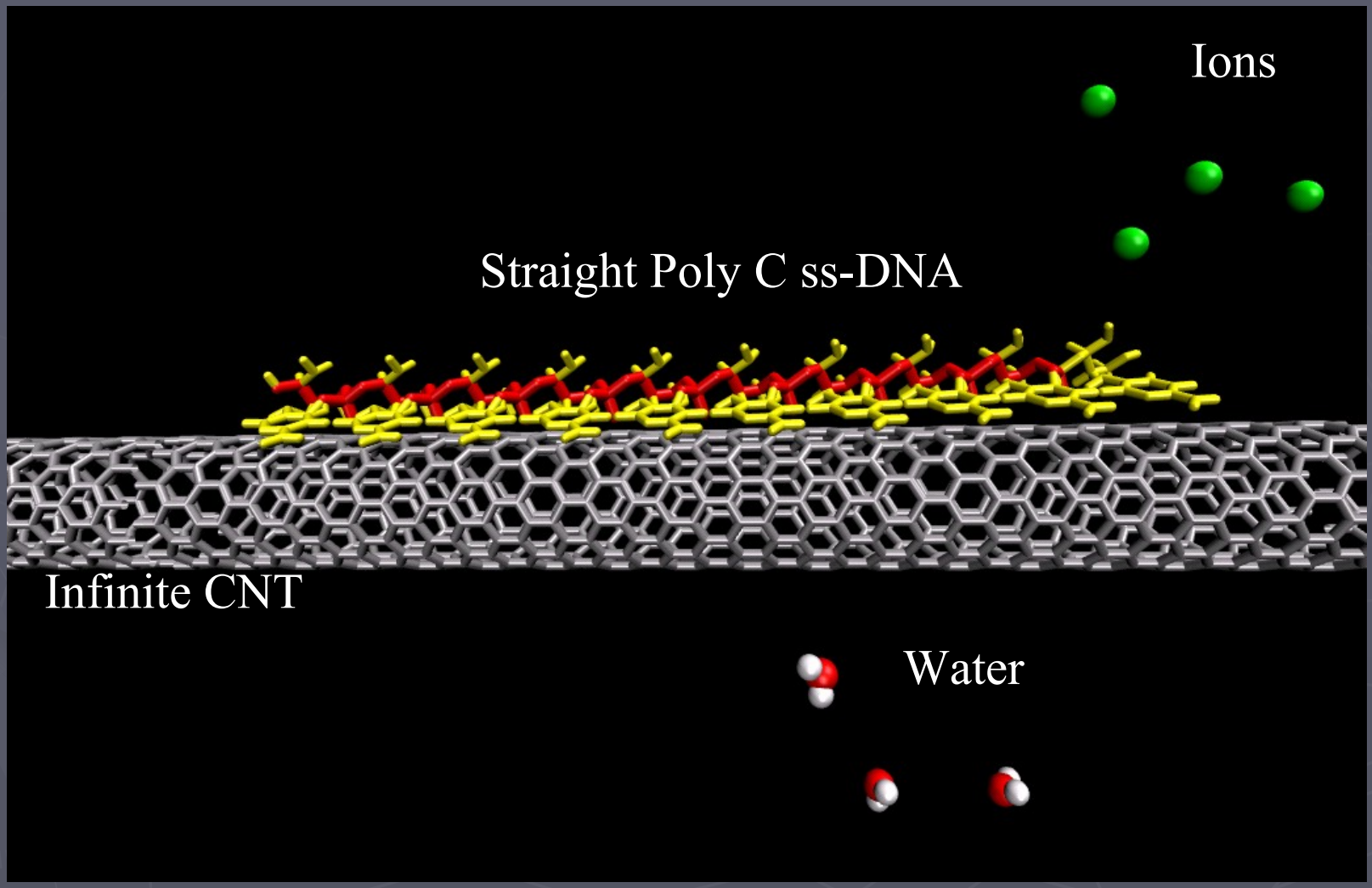
B form →



Problem

To develop methods for automatically Molecular Dynamics Simulations of Poly-C ss-DNA of different lengths adsorbing to Carbon Nanotubes.

Initial Setup

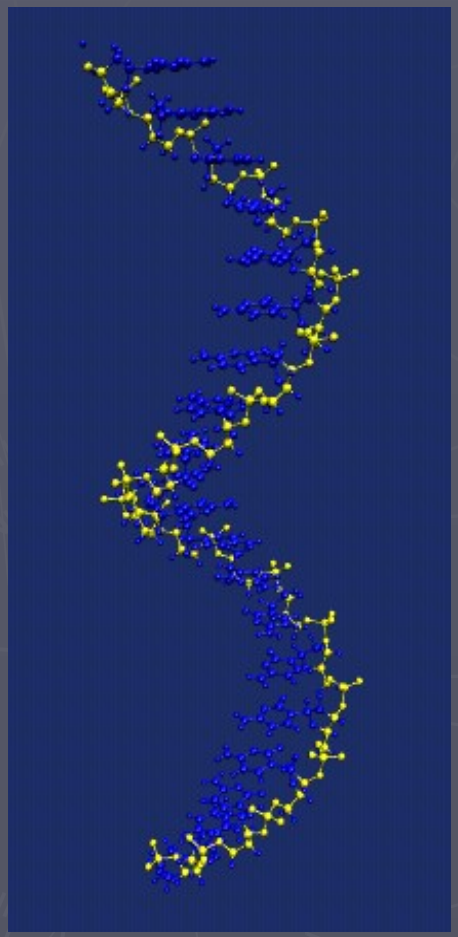


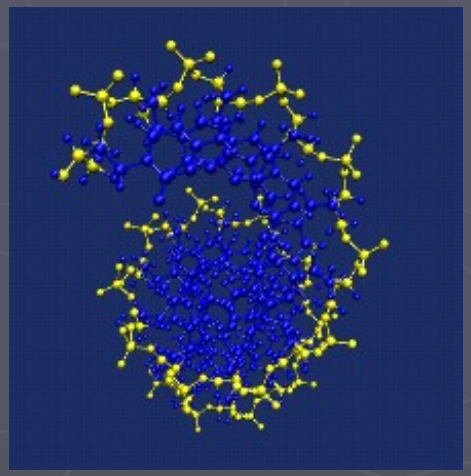
Poly C straight ss-DNA

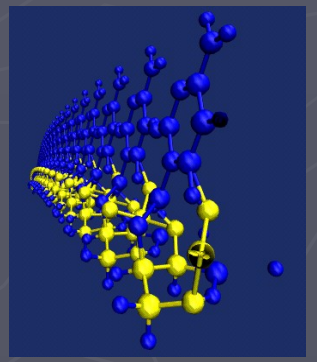
B form

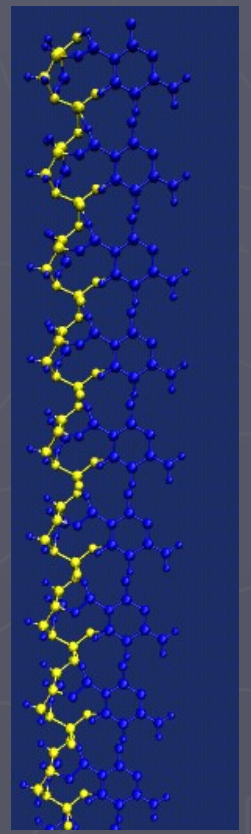
Straight form

Angles	*B-Form*	*Straight Form*
α	-46.1	161.0
β	-146.5	-289.0
γ	36.4	53.0
δ	156.5	202.0
ε	154.7	298.0
ζ	-95.6	-51.0
χ	-97.8	-141.0

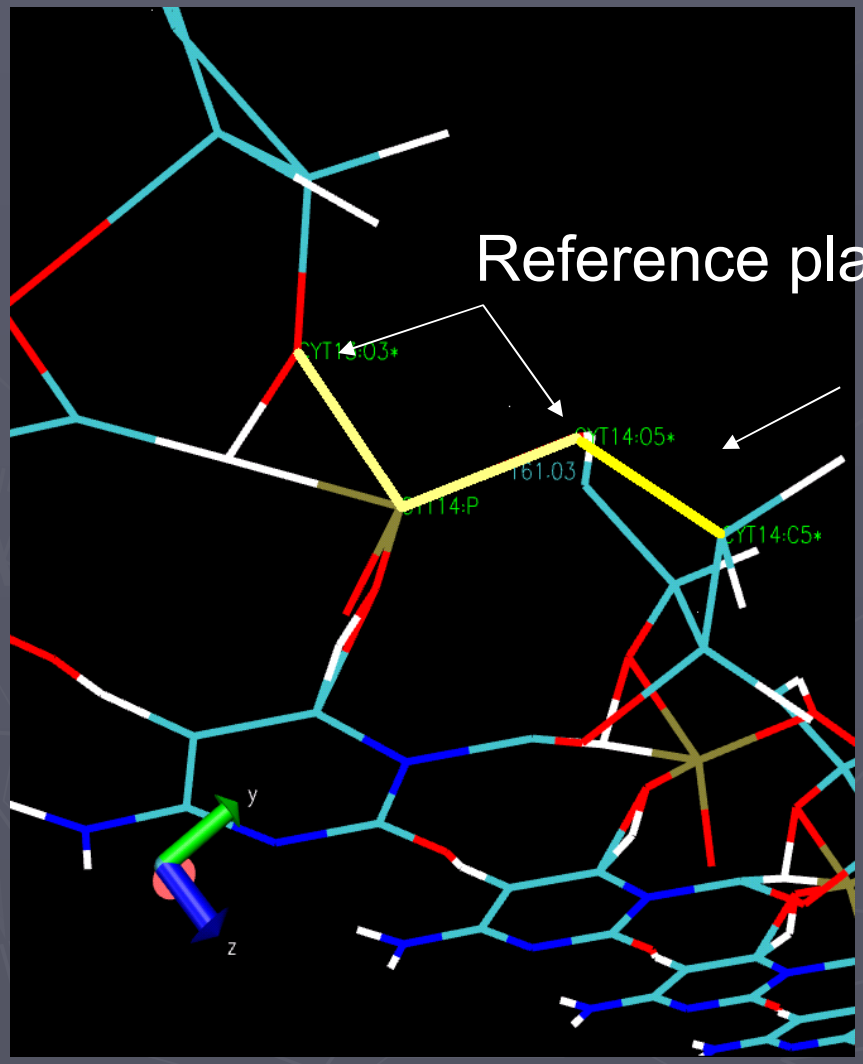








Backbone torsion angles



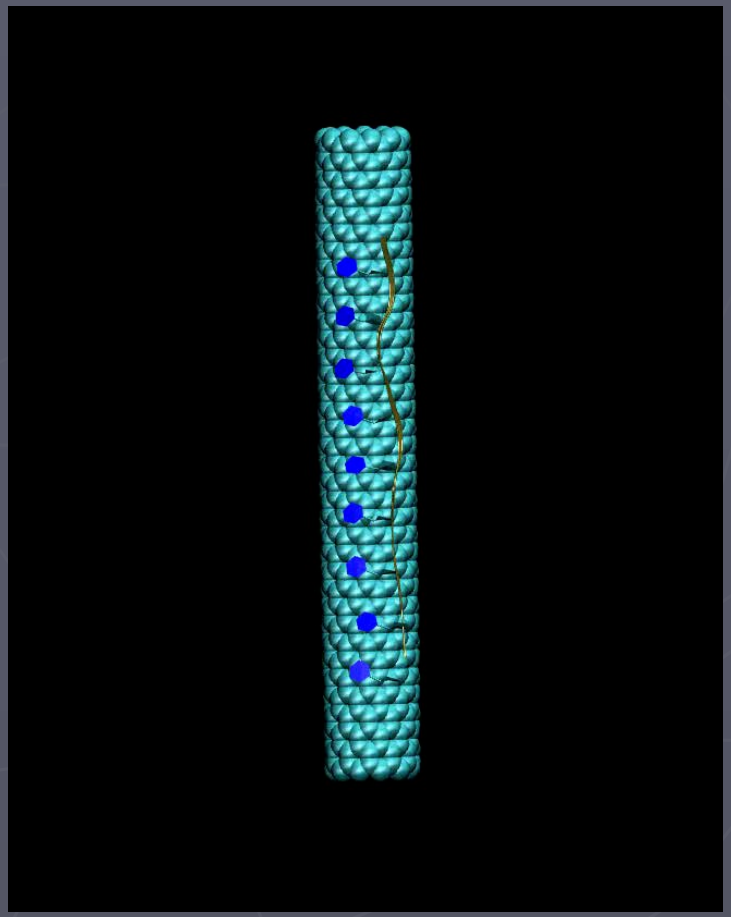
Example: α angle

Description of procedure

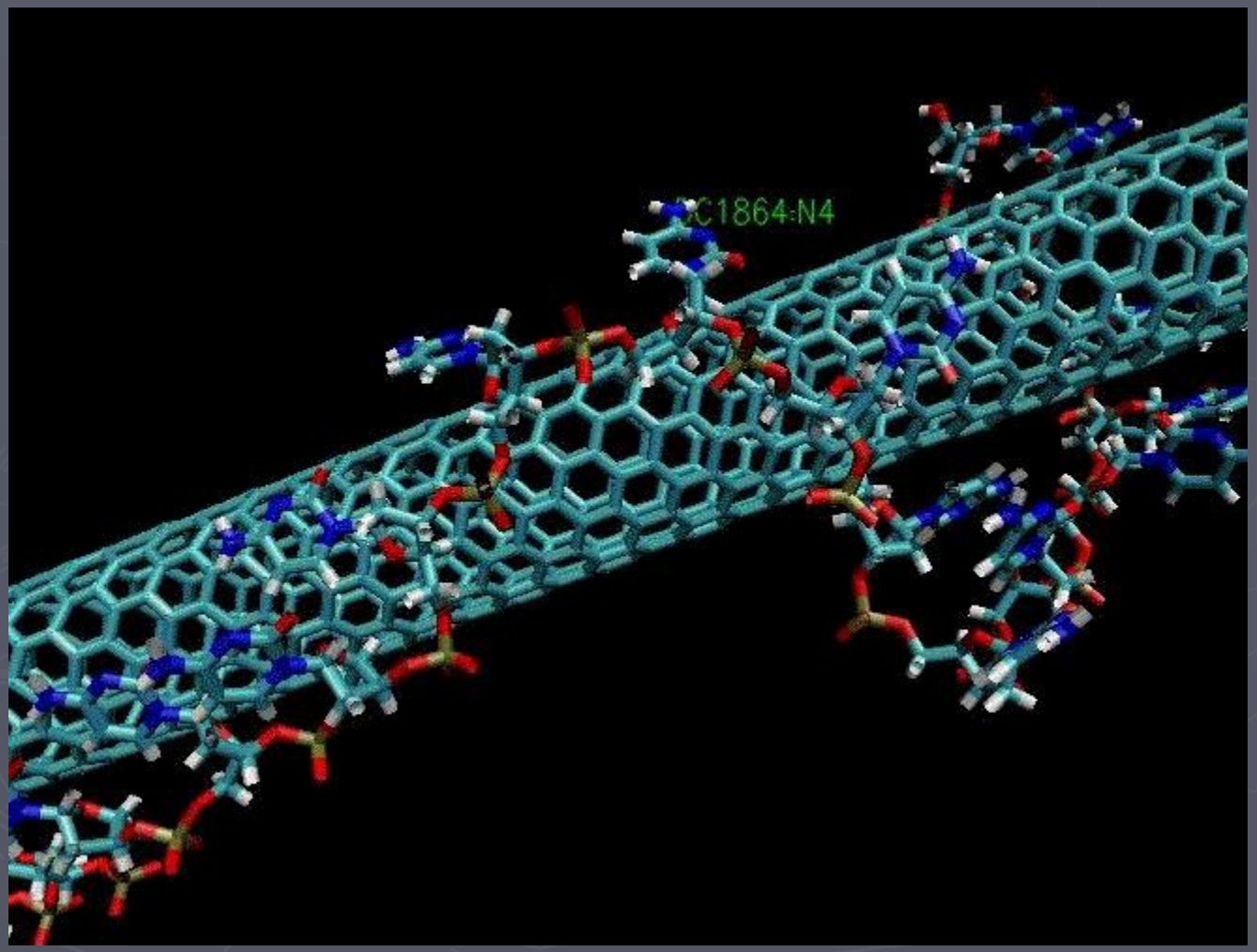
- Generate a ss-DNA of Poly C with straight conformation using **nucleic.x** (modified by us).
- Set up system with Poly-C, nanotube, solvent and ions.
- Generate the files required by the simulator.
- Run the molecular dynamics simulation via **mdrun_mpi**.
- Analyse the data produced by the simulation.

This proceduere is curently being automatized. Some editing steps require new programming in order to avoid manual manipulation of the system.

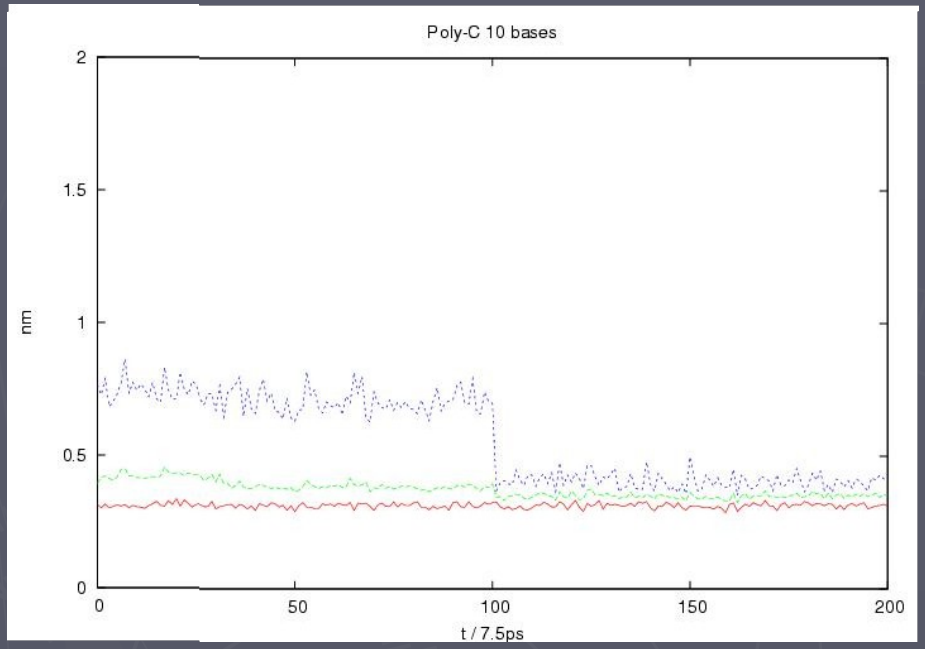
Preliminary results

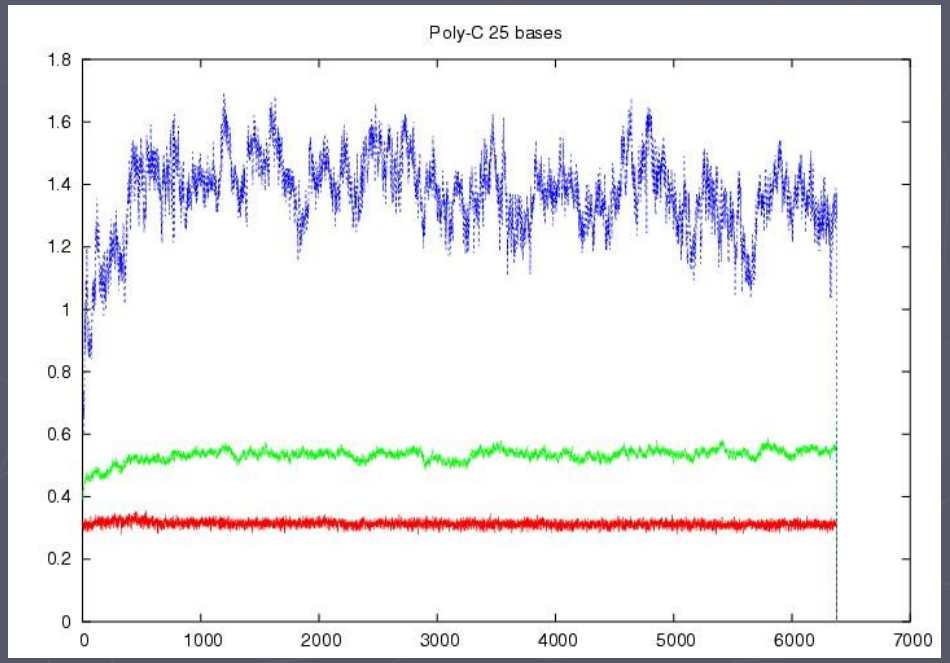


Measurement of the distance



Data analysis



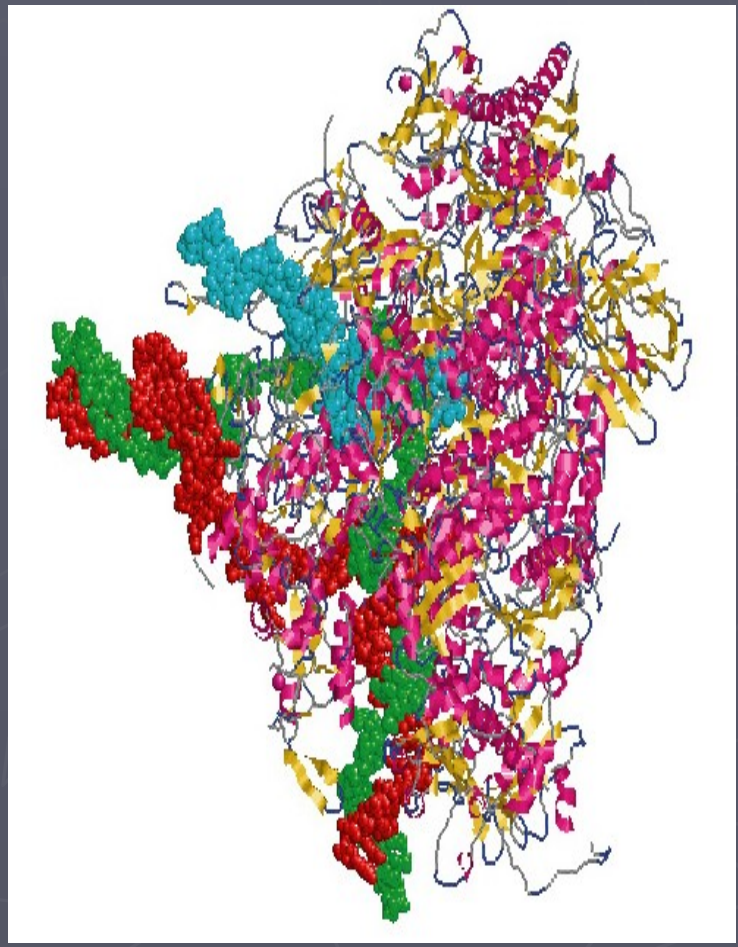


Poly-C with10 bases suggests stabilization after time.

Poly-C with 25 bases does not show stabilization after 30 times the amount of time.

Acknowledgments

To PREM Program for the opportunity to do research at the University of Pennsylvania, to the URMAA for having the best professors of the UPR-H working in research and motivating students to dedicate 100% to studies and research. To the Professor Charlie Johnson from the University of Pennsylvania for the opportunity to work with his graduate student Robert Johnson. And by finally to the Professor Jose Sotero.



Questions??

Potential

Distance between atoms i and j

Bond term

Bending angle

Bending term

Torsion angle

$$U(r_{ij}, \theta_{ijk}, \phi_{ijkl}) = K_{Cr}(e^{-\gamma(r_{ij}-r_C)} - 1)^2 + \frac{1}{2}K_{C\theta}(\cos\theta_{ijk} - \cos\theta_C)^2$$

$$+ \frac{1}{2}K_{C\phi}(1 - \cos 2\phi_{ijkl}) + 4\epsilon_{CC}\left[\left(\frac{\sigma_{CC}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{CC}}{r_{ij}}\right)^{6}\right],$$

Torsion term

Van der Waals term