TECHNION
Israel Institute of Technology
Department of Physics

COMPUTATIONAL
Physics Group

SimPhoNy

SEVENTH FRAMEWORK PROGRAMME

Simulation and vizualization of Nanotube vibrations with AViz

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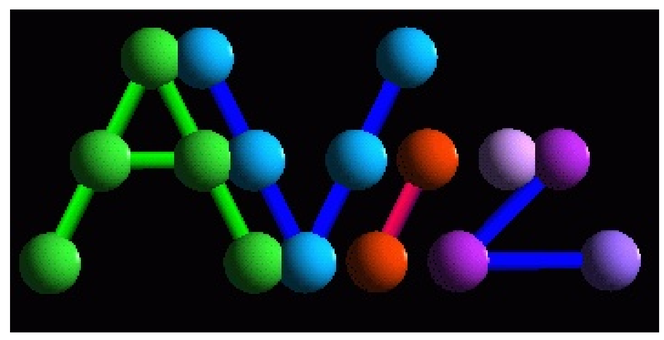
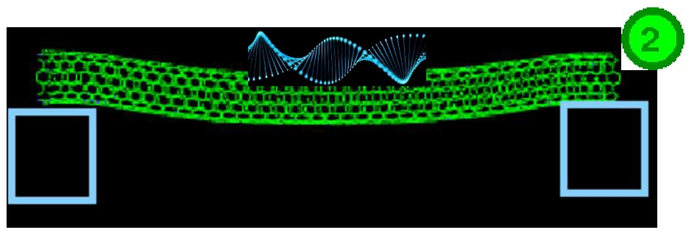
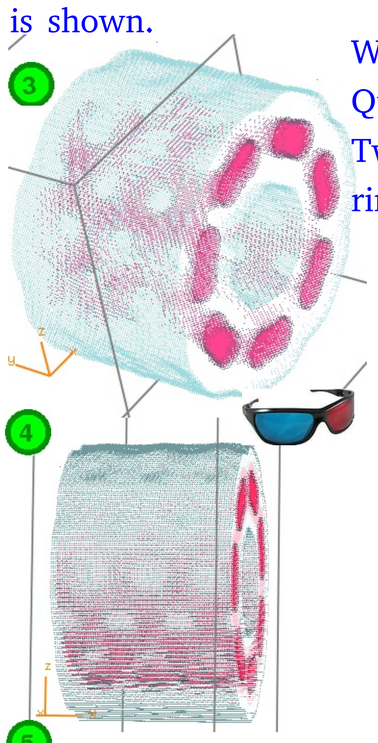
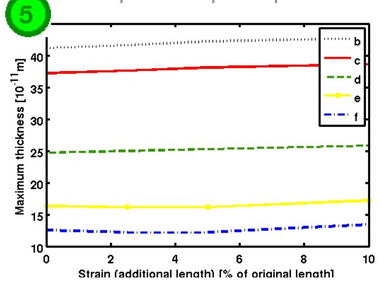


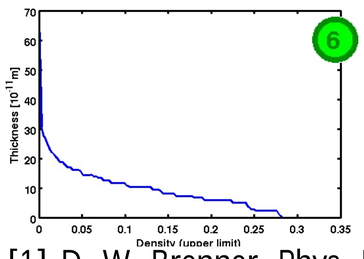
SUMMARY: One of the potential applications of the simulation and visualization techniques being developed in SimPhoNy is modelling a N(ano) E(lectro) M(echanicalystem)- a NEMS to weigh molecules such as DNA. This would be attained by calculating the change in vibrational frequency when additional mass is attached to a vibrating nanotube. The simulations of the vibrations were made with our own FORTRAN Molecular Dynamics using the Brenner potential[1], and visualizations with our AViz [2] package. To analyze the vibrations, nanotube width is an important parameter, hence we modeled the width of the electronic density envelope with AViz [3].



BACKGROUND: An image of a vibrating nanotube, from the laboratory of Y. Yaish (reproduced from [4]) is shown in Figure 1. Proof of concept was provided by Pine et al [5] who changed the mass of the nanotube's carbon atoms (by swapping for heavier isotopes and showed that the resultant change in the vibrations of nanotubes reflected the additional mass. In Figure 2 a schematic of weighing DNA is shown.



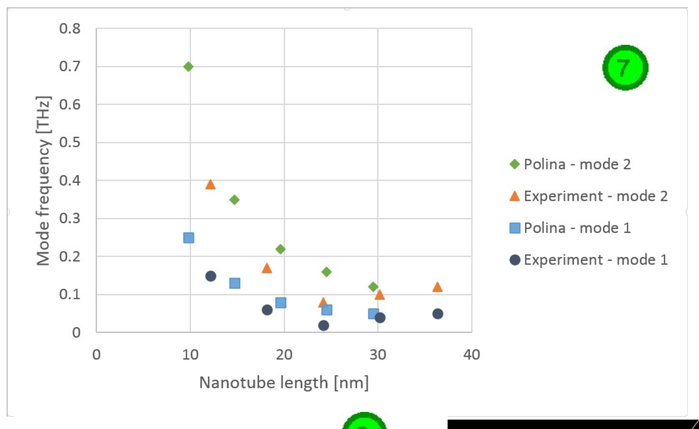




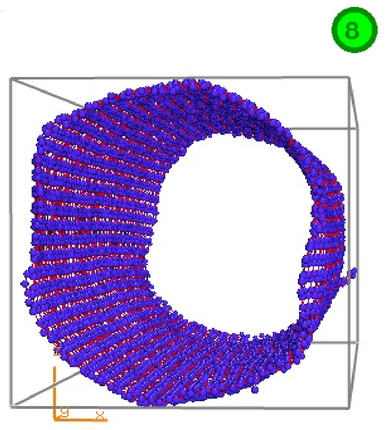
WIDTH MEASUREMENT: We used Quantum Espresso to find [6] the width. Two stereo images [7] of the width for 6 rings are shown in Figures 3 and 4.

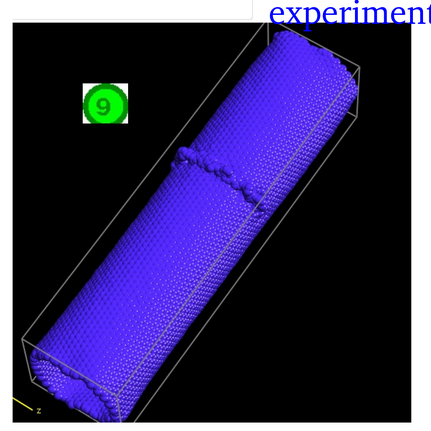
In our studies [8,9] of nanotube vibrations we found consistency with a nanotube width of about 0.07nm for the wall width, and excluded a previous estimate of .37nm. In order to confirm this directly we have taken 6 rings of a 5,5 nanotube, frozen one ring and moved the others by 2.5, 5, and 10 percent extension, similarly to those of [8]. We show [10] width as a function of tension (Figure 5), and density as a function of width (Figure 6) for the 2.5 case. The density units are as in [6], cube root of inverse Bohr radius. There is a slight increase in thickness in the stretched samples, possibly due to release of the electronic density further away.

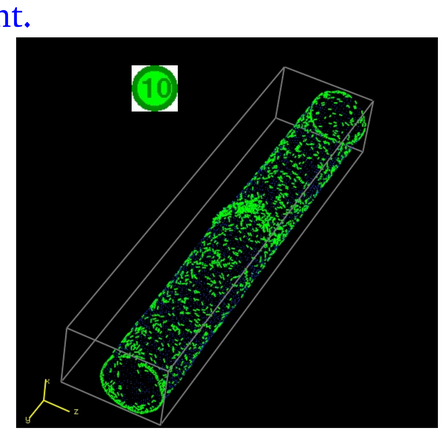
THE REAL CHALLENGE: Of course, in order to weigh attached molecules, these need to remain adsorbed on the nanotube for the time needed for the vibrational measurements. Our inital adsorbed object was selected to be ``benzene", actually a carbon ring without H atoms. Our earliest attempts to study this system were plagued by ``benzene" molecules flying off the nanotubes. Consultation with experimental students, from Y. Yaish's laboratory, led to the suggestion that a flatter nanotube may lead to an extended period of adsorption. This was indeed the case, and sucessful simulations have been made and vibrational measurements have been taken.



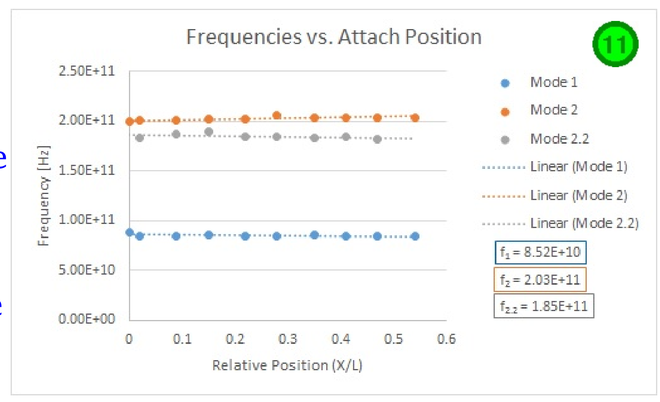
REVALIDATION: Since the new nanotubes had to be flatter and also longer, revalidation of the simulation and analysis code was done. In Figure 7 a pleasing comparison between Polina Pine's published results and the new ones is given, where the new ones are indicated by (computer) experiment.







NEXT STAGE: The benzene is shown partially attached in Figure 8 and the half ring that remained attached thruout the simulation in Figure 9. The question of where to attach the half ring was the next decision to make and in order to help decide a comparison of frequencies for different attachment points had to be taken, so a series of measurements at different points was made.



FREQUENCY MEASUREMENT: The nanotube is 310[A] in length, with a chiral vector (30,30) of armchair type, and 15060 atoms. After excluding its frozen edges (1.5 periodic rings from each edge), we are left with length of 306[A]. There are 3 half periodic rings attached (234 atoms, which are 1.55% of the nanotube mass), as an object simulating the attached molecule, see Figure 10. The additional vibrational frequency due to the attached half rings is presented in Figure 11, as a function of the attachment position along the nanotube.

CONCLUSION: It does not matter where the molucule is attached and we now have a stable system to analyze.

ACKNOWLEDGEMENTS: The latest version of AViz and the NEMS model are parts of the EU-SimPhoNy project, which has received funding from the European Union's Seventh Framework Programme under grant agreement no [604005]. The new width measurement analysis and the simulations with adsorbed objects are part of the MSc thesis project of Omri Adler.

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