Design of nanomechanical sensors based on carbon nanoribbons and nanotubes in a distributed computing system

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Software tools for *ab initio* modeling of nanoscale resonators were implemented in the GRIDIFIN infrastructure, improving the yield of the computational workload. The distributed computing system was used for the investigation of elongated edge-passivated carbon nanoribbons and nanotubes with one free end and one fixed end, by means of density functional theory simulations. Their oscillatory behavior was studied through molecular dynamics simulations. Several practical applications are envisioned for such nanostructures, such as sensors and high-frequency oscillators. The scaling of the MPI application with the number of cores was studied and the results were used to obtain the optimal number of cores on which separate instances of the code were distributed. The study was also used as an in-house benchmark of the grid system.

Keywords: nano-mechanics, oscillator, nanotube, nanoribbon, MPI application, distributed computing

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The study of nanostructures by *ab initio* and molecular dynamics (MD) methods is a good example of simulation software that lends itself well to distributed computing. These types of scientific software are usually designed in a flexible manner and can run on architectures that range from single core machines to thousands of core clusters. An example of this kind is SIESTA [Soler, Artacho, …, 2002], an *ab initio* density functional theory package that covers a large number of simulation tools that can be used to compute: electronic ground states, electronic band structures, electron densities, total and partial densities of states, electric dipole moments, Mulliken populations, spin polarized systems, atomic forces, structural relaxations, stress tensors, molecular dynamics, phonon spectra and non-equilibrium Green function transport [Brandbyge, Mozos, …, 2002]. SIESTA uses a transferable pseudopotential approximation and an efficient basis of localized atomic orbitals that speed up the computation by reducing the number of degrees of freedom involved in the simulation and also by introducing a sparse matrix in the eigenvalue problem that can be efficiently diagonalized by a numerical order-N approach.

Even though the main numerical implementation of the simulation software comes highly optimized and uses several mathematical and numerical methods for speedup, the practical execution can be further enhanced by optimizing the scientific libraries (standard, precompiled distribution libraries vs. locally compiled) and faster network communication (infiniband vs. ethernet). What we also observed is that because of the software's core algorithm (the diagonalization of large, sparse matrices) and also because of hardware limitations (mostly because inter process communication), by increasing the number of cores on which an instance runs, the simulation reaches a point of diminishing returns where the speed-up doesn't justify the additional computing power. Our empirical observation is that the optimal distribution of a single simulation run is most efficient on 8 cores, which was also pointed out by others [Huhs, 2014]. In this way, multiple independent simulations can run at once on the computing infrastructure, instead of sequentially, while also maximally benefiting from the parallel architecture.

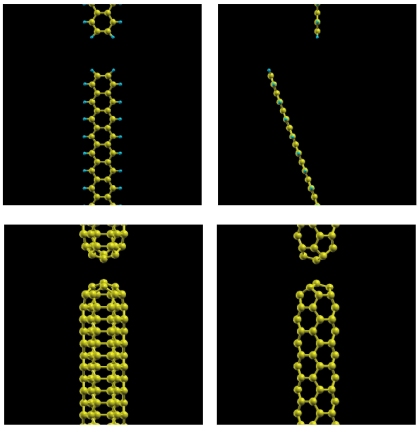

Fig. 1. Hydrogen passivated nanoribbon (top) and capped nanotube (bottom)

The systems under investigation are hydrogen passivared graphene nanoribbons and capped armchair carbon nanotubes (Fig. 1) used as mechanical resonators. Such devices are of practical interest and have multiple possible uses, such as high frequency resonators, mass spectrometer [Jensen, Kwanpyo, …, 2008], force [Sazonova, Yaish, …, 2004] and electromagnetic field [Jensen, Weldon, …, 2007] detectors or chemical sensors. The main objective was to choose the best structural configu-

ration out of the two studied by performing structural relaxation and molecular dynamics with thermostats at 150 K and 300 K.

The monolayer nanoribbon has a length of 17.3 Å and 2.8 Å in width and is made out of 32 carbon atoms and was passivated with 18 hydrogen atoms, while the nanotube has a capped end, is 35.9 Å in length and 4.2 Å in diameter and is made out of 92 C atoms. The opposite contacts for both type of structures were chosen to be similar to the resonators and are effectively extensions of them because of the periodic boundary conditions chosen. The simulation parameters were: double zeta polarized basis, local density approximation functional (LDA) and Ceperley Alder exchange correlation parametrization, 300 Ry mesh cut-off, 10^{-3} density matrix tolerance and 0.01 eV/Ang maximum force tolerance.

In order to test the structure's ability to act as nano-resonators, the nanoribbon and nanotube were first curved at an initial deflection angle (two values were testes: 10 and 20 degrees) and were then allowed to freely oscillate by performing molecular dynamics while in contact with a heath bath (canonical ensemble - Nose thermostat). In Fig. 2, snapshots from the first 3000 fs of MD for the nanoribbon are shown. The initial configuration of the bent nanoribbon was obtained by rotating the outermost two carbon atoms of the relaxed, planar structure around the attachment point (atoms at the bottom if the image) by either 10 or 20 degrees.

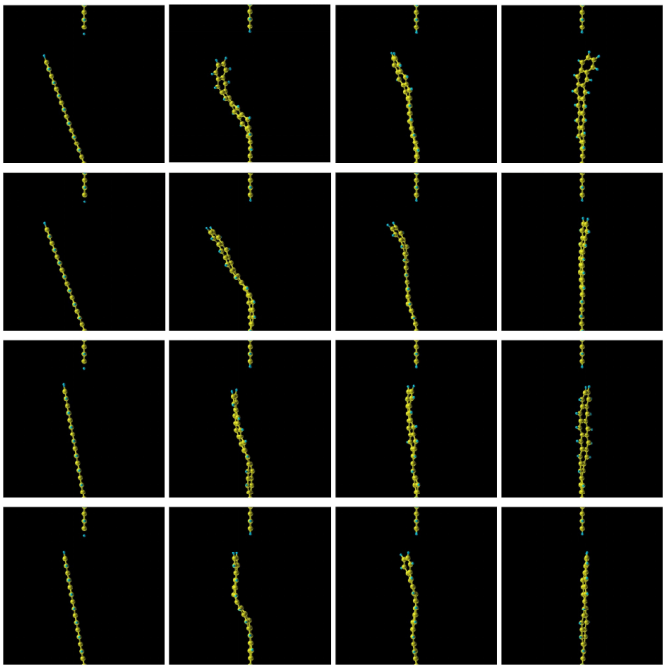

Fig. 2. Snapshots from the MD simulation of C nanoribbon taken at 0, 1000, 2000, 3000 fs - from left to right - at initial deflections of 20 degrees (for 300 and 150 K) - top two sets, and 10 degrees (for 300 and 150 K) - bottom sets

As can be seen in Fig. 2, the lack of rigidity of the nanoribbon makes it highly susceptible to thermal noise and also longer MD simulations show that this prevents it from performing meaningful oscillations. This is also visible in Fig. 4, where the position of the outermost atoms in the oscillation plane is represented as a function of time, which shows the noisy motion of the structure. The actual oscillations of the nanoribbon in longer MD simulations show to be just thermally driven, without being periodic.

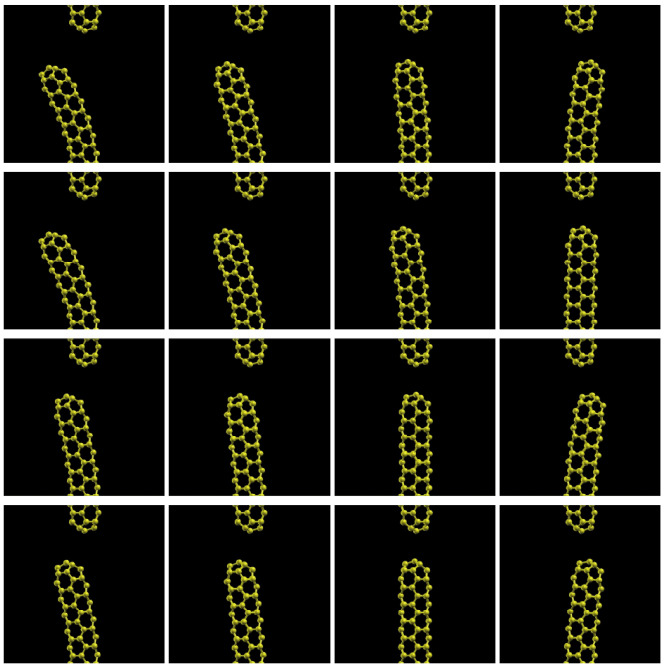

Fig. 3. Snapshots from the MD simulation of C nanotube taken at 0, 200, 400, 600 fs - from left to right - at initial deflections of 20 degrees (for 300 and 150 K) - top two sets, and 10 degrees (for 300 and 150 K) – bottom sets

The second type of structure that was investigated was a carbon nanotube with a capped end. As can be seen in Fig. 3, the oscillations of the nanotube are clearly visible. The coherent oscillatory behavior of the nanotube, seen even at 300 K (Fig. 4), shows that it is well suited as a nanoresonator.

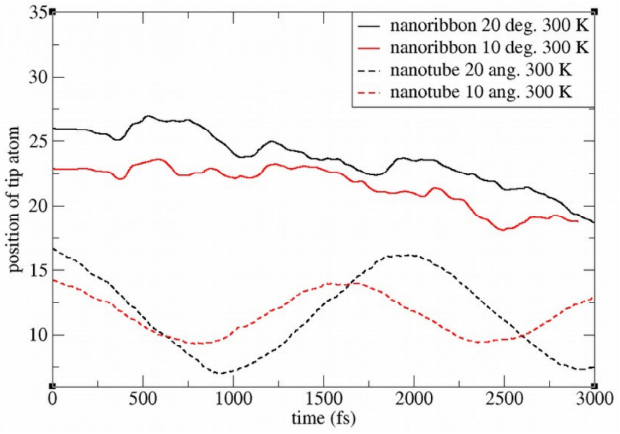

Fig. 4. Position of tip atom in the oscillation plane as a function of time for the first 3000 fs: nanoribbon vs. nanotube

As can be seen from Fig. 4, the carbon nanotube is a complex resonator, having a temperature dependent oscillation; MD simulations also show a dependence of the oscillation period with the initial deflection angle. These two observations lead to the conclusion that the small diameter nanotube functions as an anharmonic oscillator. This result is in agreement with previous studies [Fu, Hong, …, 2006; Jin, Mei, …, 2015].

We conclude that freely oscillating low diameter armchair carbon nanotubes are good candidates for mechanical resonators at the nanoscale. While having appropriate mechanical and structural prop-

erties, care must be taken when using nanotubes as sensors since they show a nonlinear behavior, depending both on temperature and deflection angle. On the other hand, freely oscillating carbon nanoribbons do not seem to be a good choice as mechanical oscillators.

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