Simulation framework for multiscale phenomena in micro and nano systems

Project acronym: **SimPhoNy (GA Nr. 604005)**

Report on Deliverable 4.1: Nano-Micro: coupling DFT-MD methods

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1 Document history

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2 Executive Summary

Electronic structure calculations based on density-functional theory (DFT) are linked to atomistic molecular dynamics simulations using the interface libraries developed in WP2 and WP1. Special focus has been given to sequential schemes (linking) and to scenarios that require repeated passage of information including interactive processing, between the DFT electronic model and its related calculation method and the atomistic model and its related methods based on empirical interatomic potentials. The focus of the work in this task is on development of a transfer protocol between the different models was done at (IIT). QuantumESPRESSO (QE) was used for the DFT and LAMMPS as well as own home-brew code for the MD part with a focus on multi-scale sequential modelling (linking) of nanotube vibrations for NEMS applications.

However the main focus in the SimPhoNy project was to provide a prototypical system on which the environment can be further developed and tested, particularly for coupling the electronic and atomistic models (IIT). The results obtained with the automated scripts in SimPhoNy were compared to those obtained manually as a validation of the linking scheme. The results have been visualized both in Aviz (IIT) and n-Cad (SG) The effort now will shift to WP5 where an application based on this coupling for calibrating NEMS devices is being developed (IIT).

Role of participants: IIT has led this task and developed the interfaces for the coupling and performed all simulations. SG has collaborated with IIT for the visualization and pre-post-processing of nanotubes with both AViz and atomistic n-CAD.

3 Contributors

- Bastien Grosso – IIT intern – original wrappers for nanotube electronic density visualization from QE results.
- Jeremy Rutman – IIT half-time researcher - SimPhoNy wrappers for nanotube electronic density visualization from QE results.
- Joan Adler – IIT – verification and development
- Omri Adler – IIT graduate student – nanotube electronic density visualization with larger nanotubes.
- G. A. Garcia, Y. Makushok, V. Makushok, J. Lama, G. Roman-Perez - SG -electronic density visualization with n-CAD

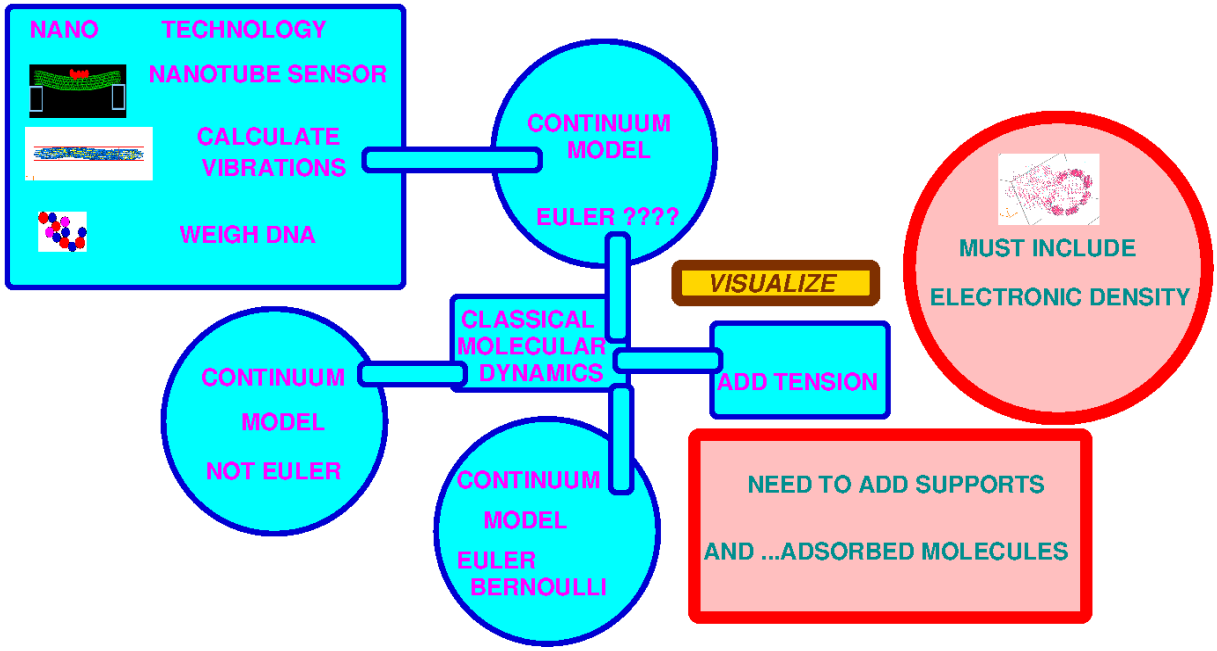
4 List of acronyms and abbreviations

QE	Quantum Espresso
DFT	Density Functional Theory
CUBA	Common Universal/Unified Attributes
CUDS	Common universal data structure
NEMS	Nano-Electro-Mechanical-Sensors
File-IO	File input and output
FVM	Finite volume method
GPL	Gnu general public license
LGPL	Lesser Gnu general public license
MML	Multiscale modeling language
MPI	Message passing interface
n-CAD	Nano scale computer aided design
SSB	Standards steering-body
TRL	Technology readiness level
UML	Unified Modeling Language
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
WP	Work Package

5 Outline of Work

As well as the general testing of wrappers and DFT-MD transfers this is the first part of the calculations needed for 5.6.

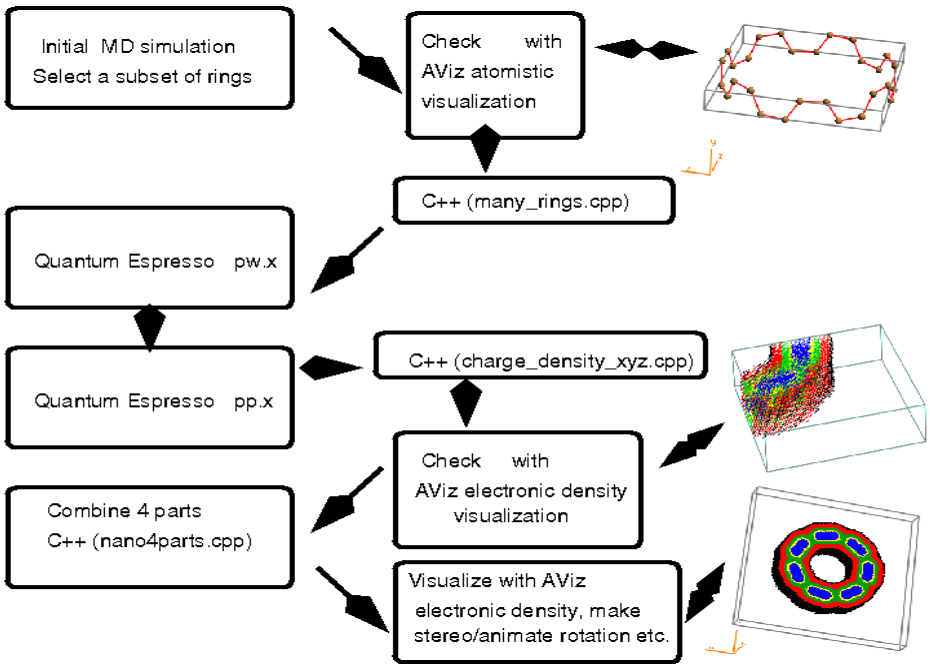
A paradigm for the project is given below:



The electronic density modelling (upper right of the above paradigm) is discussed in the next section. The supports and adsorbed molecules is in Task 5.6.

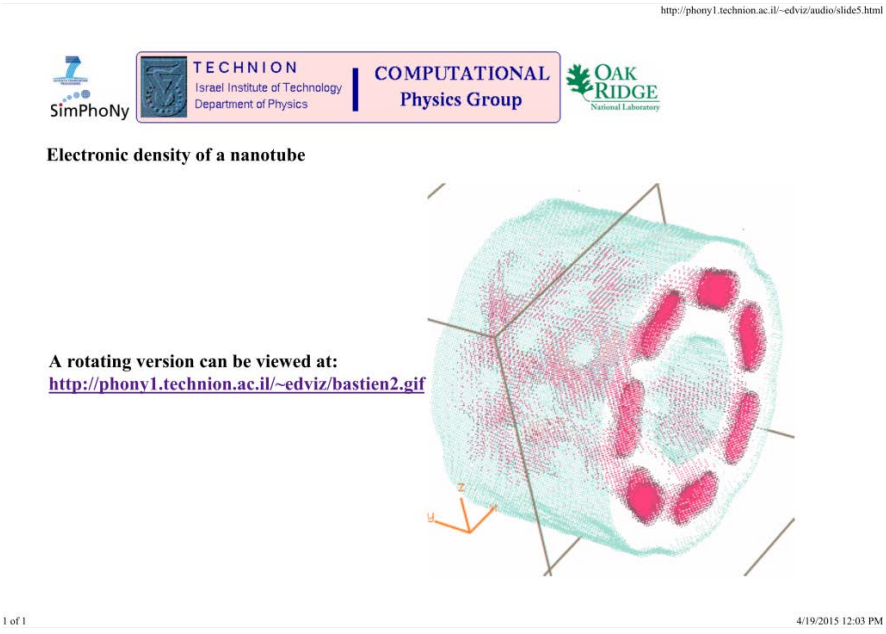
6 Electronic Density and Wrappers

The following flowchart shows the stages in the manual MD to DFT conversion.



The QE SimPhoNy, LAMMPS SimPhoNy and Aviz SimPhoNy wrappers are reported on elsewhere.

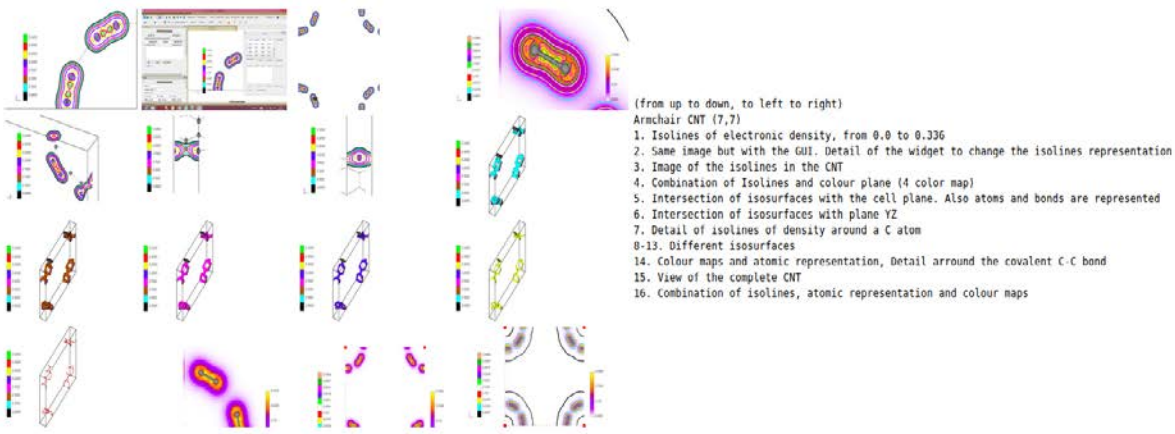
These electronic density visualizations have been reported on in several papers, and the image below is taken from one of the audio slides of one of them:



7 Electronic Density in n-CAD

One of the central SimPhoNy themes is interoperability of different codes. IIT and SGENIA have been exchanging data and images. Specific examples include SGENIA visualizations of the IIT electronic density DFT results of the nanotube simulations. The data under study are

the 1/4 nanotube rings in the datafile linked from:
http://phony1.technion.ac.il/~aviz/xyzfiles.html



This is the same data as shown in the flow chart, but with different ways to view it.

8 Publications and presentations

More technical details about the work done can be found in the following presentations and papers:

1 Visualization of electronic density" (Simphony Acknowledgement and three Simphony co-authors, Joan Adler, Adham Hashibon and Bastien Grosso), Bastien Grosso, Valentino R. Cooper, Polina Pine, Adham Hashibon, Yuval Yaish and Joan Adler. Computer Physics Communications,DOI-10.1016/j.cpc.2015.04.003 195, p 1-13 (2015).

2 ``Visualization of electronic density", Joan Adler's talk for 28th Athens, GA, USA CSP Workshop February 23-27, 2015. (Simphony Acknowledgement) that deals with AViz applications and python wrappers -50 participants.

3 Manuscript related to above talk - ``Mini-review of Visualization of electronic density" (SimpPhoNy Acknowledgement and four Simphony co-authors, Joan Adler, Omri Adler, Adham Hashibon and Bastien Grosso), Bastien Grosso, Joan Adler, Omri Adler, Or Cohen and Meytal Krief, Valentino R. Cooper, and Adham Hashibon. Physics Procedia, 68, p2-6 (2015).

4 Abstracts for INTOP2015 and for Recent Advances in Computational Modelling for Energy Applications, July, 2015, Technion. (SimPhoNy Acknowledgements, and SimPhoNy coauthors, J. Adler, O. Adler, J. Rutman, B. Grosso, A. Hashibon)

9 Summary and outlook

This stage is now complete and we are moving on to its application in Task 5.6
Some of these results will be included in a manuscript in preparation comparing the visualization approaches of SimPhoNy.