SimPhoNy

Simulation framework for multiscale phenomena in nano and micro scaled systems

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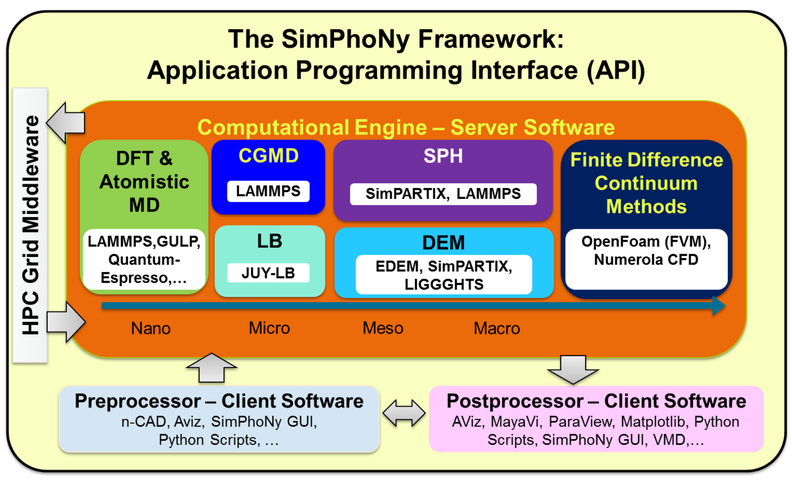
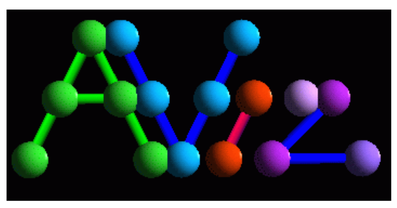
Industrial participants: DEM Solutions Ltd., UK, Enthought Inc., UK, Hellma GmbH & Co., Germany, Numerola Oy, Finland,
Sgenia Soluciones, Spain and Biofluidix, Germany





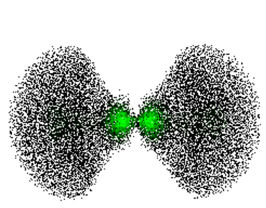
SUMMARY

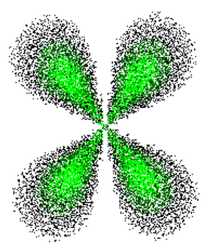
Numerous simulation methods and tools are available today for describing a material accurately and efficiently on a particular scale. The use of the various simulation tools is often hampered by a steep learning curve, which makes them unlikely to be adopted in an industrial setup. Moreover, due to the lack of coherent standardized simulation frameworks, users are expected to prepare and develop their own specialized tools to pre-process input files and build initial models, then convert simulation results into a suitable post-processing application, for example for visualization or calculation of additional properties as input for passing to other single scale tools. These operations lead to an unnecessary waste of resources and constitute a serious barrier for the broader use of nano-scale simulations.

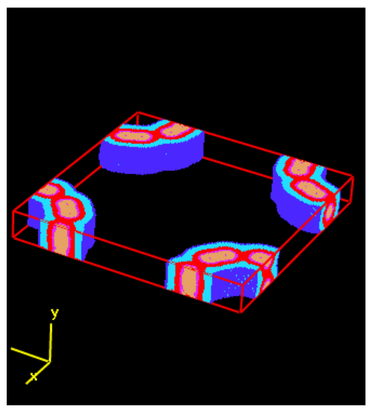
In this new EU FP7 project we will prepare a unified environment for such simulations. The Technion part (details at right) will include python interfaces to the AViz visualization package for both LAMMPS and QUANTUM ESPRESSO. One of the prototype models will be a vibrating nanotube system to be used as a mass sensor where the current molecular dynamics atomistic level of study will be extended to the electonic structure of the tube at its suspension and adsorption points. Interfaces between the atomistic and electronic scales as well as with the AViz visualization package for both levels will be created.

TECHNION PRELIMINARIES

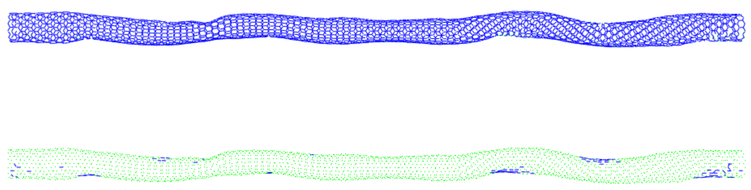
[1] AViz in offlabel dot mode for electronic structure density - Meytal Krief and Joan Adler (below left and center), 3d analglyphic steero for hydrogen atom and for DFT (Quantum ESPRESSO) for electronic density of nanotube, Valentino Cooper and Joan Adler (below right).



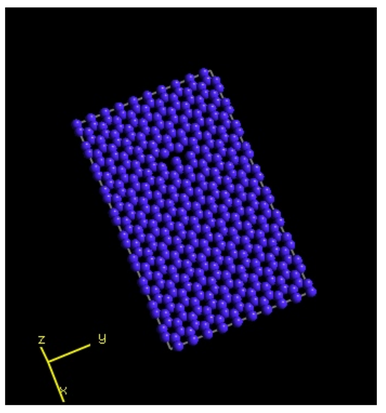




[2] AViz with own MD for nanotube vibrations - Pine, Yaish and Joan Adler (below) showing compressed bonds in lower image.



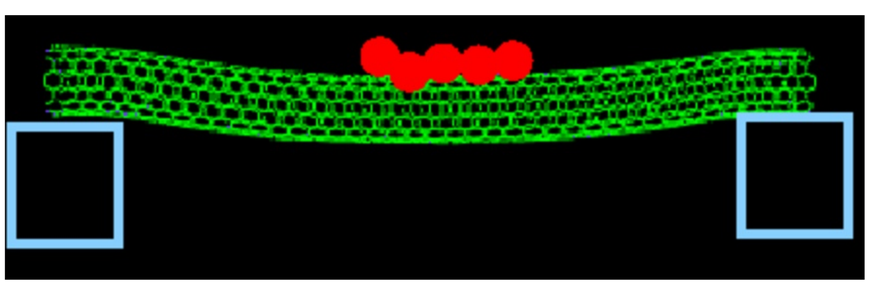
[3] LAMMPS with wrappers to AViz in C++ showing vacancies in graphene - Koren Schreiber and Joan Adler (right).



REFERENCES:
[1] J. Adler et. al. to appear in IOP Conference proceedings, http://phelafel.technion.ac.il/ ~meytal and unpublished.
[2] P. Pine, Y. Yaish and J. Adler, IOP Conference proceedings - http://iopscience.iop.org/1742-6596/402/1/012002; J. Applied Physics, 2011, Vol 110, 124311; Phys. Rev. B, 2011, 84, 245409; Phys. Rev. B, 2011, 83, 155410 and submitted.
[3] J. Adler et. al. to appear in IOP Conference proceedings, and http://phelafel.technion.ac.il/~korens/project.html

PROTOTYPE

Green - vibrating nanotube
Red - adsorbed molecule
Blue - supports



TECHNION TO DO

Repeat above with python wrappers.
Make DFT study of nanotube suspension supports and nanotube.
Make DFT study of adsorption of molecules to nanotube.
Elucidate full prescription for when continuum approximations for nanotube vibrations valid.

Now HIRING a programmer, and interviewing potential postdoctoral fellows and graduate students.
See http://phycomp.technion.ac.il and contact Joan Adler at phr76ja@tx.technion.ac.il or at 048293937.