Simulation framework for multiscale phenomena in micro and nano systems

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

Report on Deliverable 6.4: Educational Resources

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1 Document history

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21.04.2015	*V0.1*	*Joan Adler*	*Initial version*
27.04.2015	*V0.2*	*Adham Hashibon*	*Review and incorporation of text*
27.04.2015	*V1.0*	*Joan Adler*	*Review references and web links, final review*

Contents

2 Executive Summary

In *Task 6.1 – Dissemination of result,* the aim of the SimPhoNy project is to create a new educational computational science and engineering resource with a special emphasis on Nanotechnology and especially on multi-scale approaches. This is intended to provide educators and students online resources through a simple web-site that allows students and educators to explore the capabilities of multi-scale science, and to easily set up and run test educational cases.

We have set up educational tools for students at both undergraduate and graduate level complemented by a Computational Physics education page [1] currently in development on the C20 website to provide more emphasis on Nanotechnology applications. This is achieved through visible links on the project web-site and other dissemination activities in WP6. The website will be continuously updated by the partners with additional use cases and educational applications based on the work done in WP4 and WP5 using the SimPhoNy simulation environment and make them, along with description of the multi-scale science, available on this educational resource.

Eventually as the SimPhoNy framework becomes mature enough (includes the integration of the Middleware solution and client server architecture, expected in M26 and M27), interactive web-interfaces will also be provided to help set up modelling cases for educational purposes.

3 Contributors

- IIT collected a number of education cases also from various partners.

4 List of acronyms and abbreviations

API	Application programming interface
CUBA	Common Universal/Unified Base Attributes
CUDS	Common universal data structure
DEM	Discrete elements method
DFT	Density functional theory
FEM	Finite elements method
File-IO	File input and output
GPL	Gnu general public license
LGPL	Lesser Gnu general public license
MD	Molecular dynamics
SPH	Smoothed particle hydrodynamics
SSB	Standards steering-body

TRL	Technology readiness level
LB	Lattice Boltzmann
WP	Work Package

5 SimPhoNy educational resource

The ability of European Nanotechnology industries to unravel their full potential by turning fundamental research into successful innovations hinges on the availability of highly knowledgeable and well trained scientists and engineers, who are also able to apply and understand multi-scale paradigms in the design of novel applications. Education in Computational Science and Engineering is a fairly new endeavour. Physics education is now a mature field, but Computational Physics education is fairly new. Education for Nanotechnology students is even newer, not surprising since Nanotechnology as a discipline is also new.

Our aim in SimPhoNy project is to create a new educational computational science and engineering resource with a special emphasis on Nanotechnology and especially on multi-scale approaches.

We have started a website with a collection of nanotechnology simulation and educational resources. Computational Physics or Engineering Education is relatively well established fields, with sections and columns in several Journals, such as Computational Science and Engineering of the US IEEE and AIP. Computational Nanotechnology is much newer and Computational Nanotechnology Education newer still. Of course, there are many overlaps, especially with Computational Chemistry Education, and High Performance Computing training such as that done in the European context by PRACE. Many existing initiatives were described in our proposal, and we began a process of selecting and referencing those most relevant for multiscale nanotechnological computations, with an emphasis on educational material for the codes that form parts of the SimPhoNy project. Figure 1 shows a snapshot of the main page of the SimPhoNy Educational Resources website (taken on 27.4.2015). The website is currently hosted at IIT under the web-address:

http://phony1.technion.ac.il/~simphony/list/edres.html

(Sim)phony1 is one of the servers acquired by the SimPhoNy project (hostname regulations at IIT require names of computers situated in the physics department to start with ph).

A list of articles and course material for general Computational Physics education has been made by IIT as part of the IUPAP C20 Computational Physics website, but this covers physics in general. We have begun a more specific listing for nano and multiscale approaches, currently under development at the Educational website above. This is due to be moved to the official SimPhoNy site when a little more mature. Its current form is a set of links to educational websites at three levels:

1. High School enrichment (and University open days),

2. Undergraduates and
3. Graduate students and researchers.

The IIT websites are mainly produced by undergraduate and graduate students in Computational Physics classes or as undergraduate or summer intern projects. Thus both the student writer and the later student readers benefit. Note that the projects selected to be linked here were created by students from physics, chemistry, computer science, mechanical, civil and electrical engineering and nanotechnology programs.

Many of the projects include instructions for creating output files that can be graphed by AViz (http://github.com/simphony).

Future plans include in-depth and beginners Lattice Boltzman tutorial from JYU, instructional material for other codes in use in SimPhoNy, and of course incorporation into the official site. We also plan to publicize some outreach material focused on nanotubes suitable for quite young high schoolers.

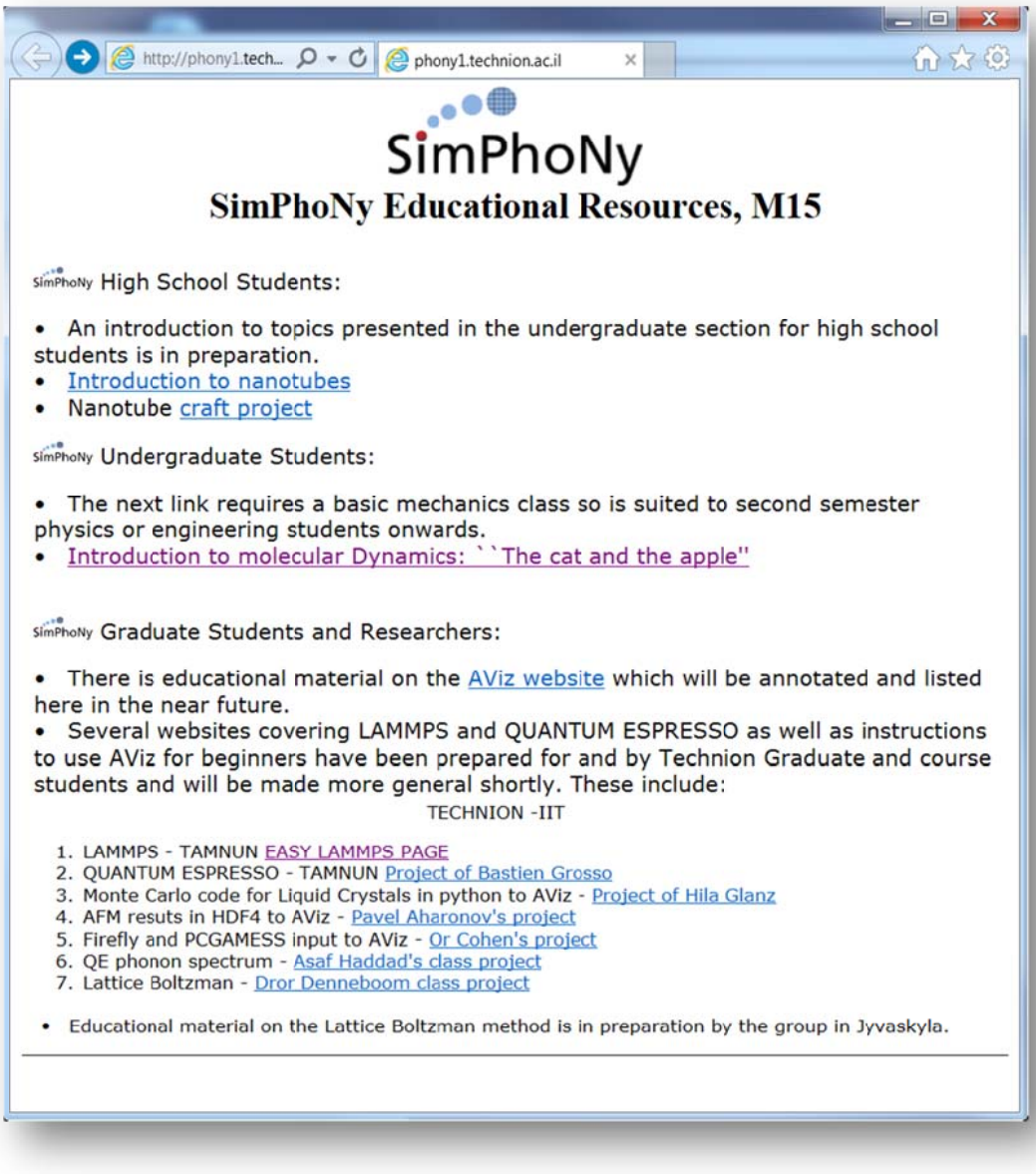

Figure 1 A snapshot of the SimPhoNy Educational Website from 27.4.2015, shoing main structure and links to various topics. Site can be visited under: http://phony1.technion.ac.il/~simphony/list/section3.html

6 Next Steps

Further contributions will be made from several partners, including:

- Links to official SimPhoNy documentation which is situated at http://simphony.readthedocs.org/en/stable
- LB tutorial from JYU
- MD tutorial from IWM
- Post and Preprocessing with nCad and nCad-Fluid from SG
- Post and Preprocessing with VTK based tools (IWM, ENT)
- Tutorials for installations and use cases for all wrappers in SimPhoNy (An extremely preliminary start to this is taking shape at: http://phony1.technion.ac.il~simphony/tutorials/tutorials.html)

7 Summary and Outlook

A first public release of the SimPhoNy Educational Website has been completed; the website from this point on will evolve and include further case studies and links to the documentation pages of SimPhoNy.

8 Licensing status

Not applicable.

9 References

[1] http://phycomp.technion.ac.il/~C20/education.html