



# Simulation framework for multiscale phenomena in micro and nano systems



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

## *Report on Deliverable 6.5: Training week: European Workshop 2 - topic: Training week for students*

<b>Document Version:</b>	<i>V0.1</i>
<b>Dissemination Level:</b>	<i>PU</i>
<b>Related Tasks</b>	<i>Task 6.1: Training Week</i>
<b>Deliverable due:</b>	<i>M24</i>
<b>Submitted:</b>	<i>M30</i>
<b>lead beneficiary:</b>	<i>IIT</i>
<b>Contributing partners:</b>	
<b>Status:</b>	<i>Final</i>





# 1 Document history

<b>Date</b>	<b>version number</b>	<b>Author</b>	<b>Comments</b>
<i>28.06.2016</i>	<i>V0.1</i>	<i>Joan Adler</i>	<i>Based on M24 minutes report</i>
<i>29.6.2016</i>	<i>V1.0</i>	<i>Adham Hashibon</i>	<i>Review and Submission</i>



## 2 Executive Summary

SimPhoNy includes two workshops and a training week for students with the aim of user teaching as described in WP6. Since SimPhoNy has already participated in organisation of a number of workshops that include training (example, the CECAM workshop in September) and in order to avoid overlap the focus of the workshop in D6.5 was shifted to students and focused on those from within the partners as well as from the hosting institution (IIT). The workshop took place at the Technion, Israel Institute of Technology and was adjunct to the M24 General Assembly meeting. The Agenda of the M24 meeting contained therefore additional open sessions (see attached agenda). On the second day, a hands-on session was organised. A number of workstations were provided for partners. The client server architecture was demonstrated for the first time. In addition partners exchange information and practical expertise installing and demoing various wrappers.

On Day three, an open session was conducted open to external participants, that was advertised to the Nanotechnology Institute and other Technion researchers. Some 30 participants from Physics, Chemistry, Mathematics and Mechanical and Electrical Engineering attended a presentation by Guillermo Roman from Sgenia about NCAD, NCAD fluid and SimPhoNy. This was followed by additional hands on session, and a SimPhoNy only SSB/DevTeam Meeting on the metadata schema.

Efforts from this WP and task are also shifted towards the planning of the workshop : Multiscale Simulation: from Materials through to Industrial Usage, supported by CECAM-IRL, September 5-9, 2016 in Dublin where Joan Adler (IIT) is a co-organiser and several from SimPhoNy will contribute to the talks and the hand on plug-fest (Fraunhofer, IIT).

### Contributors

- IIT organised the session and provided all workstations
- JYU, QNT, Fraunhofer and BFX assisted the organisation and provided additional discussions and tutorials.

## SimPhoNy M24 Meeting Agenda

**Data and time: Monday 25.01.2016, 09:00 – Thursday 28.1.2016 14:00**

**Venue:** The Physics Department, Technion City, Haifa, Israel.

All activities will be in the Seminar Room No. 620.

**Participants: see attached scan of signed participants lists**

**Additional remote participation:** Pooyan Dadvand (QNT), Mehdi Sadeghi (IWM), Kit Choi and Didrik Pinte, (ENT), Oscar Paz (SG)

### Day 0: Monday 25.01.2016, 16:00-19:00

**Preliminary session:** computer installation and plug fest preparation, dissemination discussions (in the Seminar Room 620)

### Day 1: Tuesday 26.01.2016, 09:00-17:00

**08:30** Registration and reception

### ***Session 1: Introduction and General Items***

**09:00** **Brief Introduction, welcome and presentation**

Professor Anath Fischer, Deputy Executive Vice President for Research, Technion.



**09:15**      **Opening, project status, administrative and financial issues including first periodic report and midterm review meeting**  
*Adham Hashibon (IWM)*

**09:45**      **Dissemination activities**  
 Workshops, meetings and training activities  
*Joan Adler (IIT)*

**Session 2: WP1 & WP2 - API & Integration, Implementation of Interface Wrappers**

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**10:00**      **Status of the SimPhoNy framework Specifications: D1.3 and D1.6**  
 CUDS as the SimPhoNy Computational Model using the Terminology of the RoMM.  
*Adham Hashibon (IWM), Kai Hiltunen (NUM), Keijo Mattila (JYU), Guillermo Román-Pérez (SG), Pooyan Dadvand (QNT)*

**10:40**      **Particle Based Wrappers (Discrete Models)**  
 File-IO and Internal Wrappers: current status, needs, and outlook plan  
*Adham Hashibon (IWM), Miguel Ángel Celigueta (CIM), Guillermo Román-Pérez (SG), Carlos Roig (CIM), Gregorio Garcia (SG), Pooyan Dadvand (QNT), Jeremy Rutman (IIT), Joan Adler (IIT)*

**11:20**      **Short Break with Coffee & Tea**

**11:30**      **LATTICE Based Wrappers (Continuum Models)**  
 File-IO and Internal Wrappers: current status, needs, and outlook plan  
*Keijo Mattila (JYY), Puurtinen Tuomas (JYU), Jari Hyväluoma, Kulju Sampo (LUKE)*

**12:10**      **MESH Based Wrappers (Continuum Models)**  
*Kai Hiltunen (NUM), Janne Martikainen (NUM), Carlos Roig (CIM), Pooyan Dadvand (QNT), Miguel Ángel Celigueta (CIM), Gerardo Socorro (QNT), Norberto Marcelo Nigro Sardella (CIM), Juan Marcelo Gimenez (CIM)*

**12:50**      **Lunch**

**Session 3: WP4 & WP5, Development of Multiscale Science (Coupling and Linking) and Validation**

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**14:00**      **Overview of Scientific Tasks and General Update**  
*Adham Hashibon (IWM), Keijo Mattila (JYU), Kai Hiltunen (NUM), Joan Adler (IIT)*

**14:10**      **Task 5.1 – Experimental determination of physical properties of complex fluids & Task 5.2 – Nano-printing Experimental benchmarks**  
*Lutz Rigger (BFX), Peter Koltay (BFX), Seoung-Eun Kim (HEL), Melanie Bruch (HEL), Keijo Mattila (JYU), Adham Hashibon (IWM), Tobias Rasp (IWM)*



- 14:50**      **Tasks 4.1 - Nano-Micro coupling: DFT-MD & Task 5.6 – Proof-of-principles Design tool for NEMS**  
*Joan Adler (IIT), Guillermo Román-Pérez (SG), Omri Adler (IIT)*
- 15:30**      **Task 4.2 – Nano-Micro-Meso: coupling of CGMD with LB/SPH & Task 5.3 – Design tool for nano-printing applications**  
*Keijo Mattila (JYU), Jari Hyväluoma (LUKE), Tobias Rasp and Adham Hashibon (IWM)*
- 16:10**      **Short Break with Coffee & Tea**
- 16:20**      **Task 4.3 – Nano-Meso-Macro: coupling DEM-(LB)-CFD & Task 5.7 – New optimized foam-forming process for biodegradable materials**  
*Kai Hiltunen (NUM), Pooyan Dadvand (QNT), Gerardo Soccoro (QNT), Miguel Ángel Celigueta (CIM), Keijo Mattila (JYU), Guillermo Román-Pérez (SG), Gregorio Garcia (SG)*
- 17:00**      **Task 4.4: Nano-Meso: coupling MD-CFD & Task 5.4 – Design tool for bubble-free nano and microfluidic applications**  
*Tobias Rasp (IWM), Nathan Franklin (IWM), Adham Hashibon (IWM), Guillermo Román-Pérez (SG), Gregorio Garcia (SG)*
- 17:40-18:00**      **Summary and Open Discussion**
- 19:00- 21:30**      **Networking Dinner with Fluid dynamics and Interoperability Discussions!**

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**Day 2: Wednesday 27.01.2016, 09:00-16:00**

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**Session 3: WP3, Pre/Post Processing, client-server**

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**09:00-09:10**      **Registration**

- 9:10**              **The n-CAD Fluid preprocessor for particle and mesh based simulations of fluids**  
*Guillermo Román-Pérez (SG)*
- 9:50**              **Developing an efficient atomistic visualization and pre-processing tool: AViz and n-CAD for Atomistics.**  
*Joan Adler, Jeremy Rutman (IIT), Guillermo Roman-Perez (SG)*
- 10:30**              **Short Break with Coffee & Tea**
- 10:40**              **Interfacing and development of VTK-based tools with SimPhoNy and the visualization interfaces**  
*Kit Choi , Ioannis Tziakos, Didrik Pinte (ENT)*
- 11:20**              **Client-Server architecture**



*Adham Hashibon (IWM), Mehdi Sadeghi (IWM), Pooyan Dadvand (QNT), Gerardo Soccoro (QNT), Didrik Pinte (ENT), Ioannis Tziakos (ENT), Kit Choi (ENT), Jeremy Rutman (IIT), Joan Adler (IIT), Amihai Silvermann (IIT)*

**12:00 Lunch**

***Session 4: Demonstration and hands-on Session***

*(At least one Ubuntu 14.04 workstation and laptop 12.04 with VirtualBox will be available)*

- 12:30** Electronic Model Wrappers (IIT), Jeremy Rutman
- 13:00** Particle Model Wrappers (IWM, IIT, CIM, QNT)
- 13:30** Continuum Model Wrappers (including LB) (NUM, QNT, CIM, JYU)
- 14:30** Client Server and pre/postprocessors (Aviz, nCAD, Mayavi, Paraview)

***Session 5: 15:00 – 15:30 Summary and Open Discussion***

*All Participants:*

- Focus on Applications and Validation in the second period
- Action plan for the next six months
- Dissemination plans
- SimPhoNy continuation, existing suitable calls (EMMC)

**15:30 Final Remarks**

*Adham Hashibon and Gerhard Goldbeck*

**16:00 -17:30** *Open hands on exchange and additional demos and development interaction time*

**Day 3: Thursday 28.01.2016, Open SimPhoNy Demo and Training**

*This is not part of the closed project meeting. It is a dissemination activity open to external participants and organized by Joan Adler (IIT).*

- 09:45** Coffee and Registration
- 10:00-11:30** – Presentation by Sgenia of NCAD and N-Fluid
- 11:30-12:00** – Panel discussion on visualization and demos
- 12:00** – Lunch with Discussion about meeting in Ireland (CECAM)