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PROJECT FINAL REPORT

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Project acronym: SimPhoNy

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4.1 Final publishable summary report

Executive summary

SimPhoNy advances the state of the art of multiscale nano-enabled materials modelling by contributing significantly to reducing the gap between materials modelling and European nanotechnology industries by developing an easy-to-use, freely available, integrated and multiscale modelling environment for nano-enabled materials and systems by design (see Figure 1). Specifically, SimPhoNy significantly reduces the number of operations and efforts needed to develop advanced modelling applications, leading to significant savings in efforts and optimal use of R&D resources and decreasing the barrier for the broader use of advanced integrated modelling workflows and multi-scale simulations in European industry.

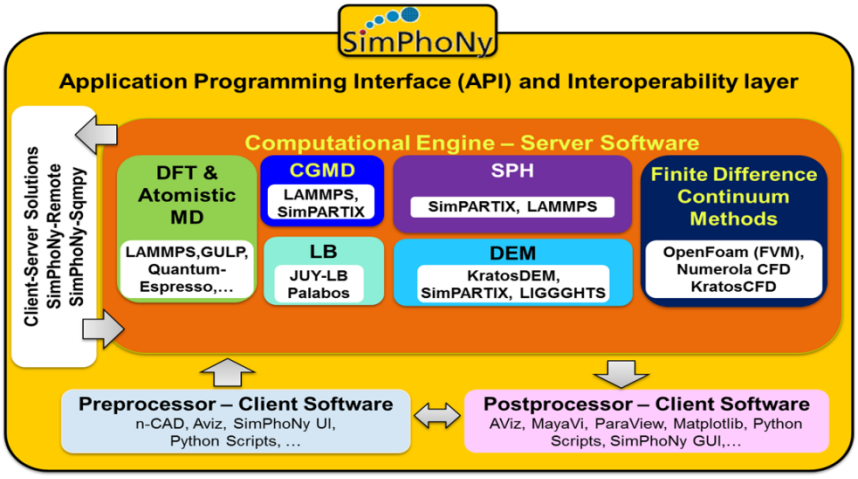


Figure 1: The main SimPhoNy integration concept and some of the tools integrated.

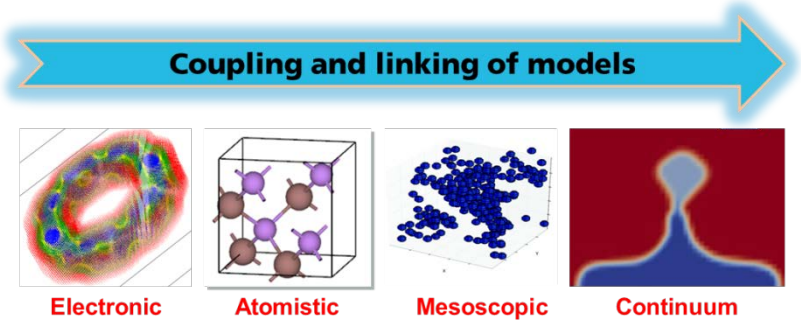


Figure 2: Materials exhibit intertwined behaviour on multiple scales requiring integrated materials modelling

Materials exhibit intertwined and inter-linked phenomena on multiple levels and scales (Figure 2), requiring thus a combination of various models into multiscale and integrated materials modelling workflows to achieve a reliable accurate description of material behaviour, especially for nano-enabled applications. Such integration requires interoperability, i.e., the seamless exchange of information between all models applied on all scales. The SimPhoNy project addresses precisely this aspect by developing an integrated simulation environment that provides for complete interoperability between models and their respective tools (Figure 3), allowing thus advanced materials modelling workflows integrating arbitrary number of models operating on various scales. SimPhoNy allows reusing existing well established simulation tools as building blocks for sophisticated workflows based on common data structures and application programming interfaces. Ontology based metadata schema is developed to bridge both the technical and terminology gaps between different

modelling communities. The integrated simulation environment is then applied for a cluster of technologically relevant applications demonstrating its capabilities, especially for the rapid development of advanced multiscale materials modelling workflows incorporating electronic, atomistic, mesoscopic, and continuum models together with advanced pre and post processing.

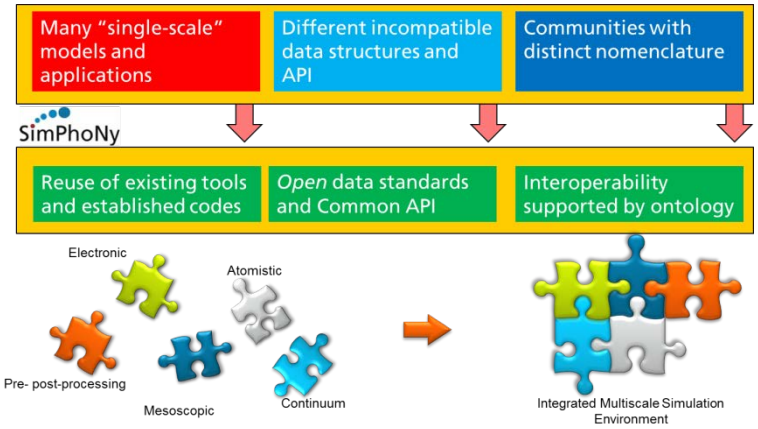


Figure 3: The main approach of SimPhoNy reusing existing well-established simulation tools, augmenting them with data standard interface layers to achieve interoperability and tight integration allowing developed of Integrated Materials Modelling Workflows, including multiscaling.

A summary description of project context and objectives

The steady progress in the various fields of materials modelling, electronic, atomistic, mesoscopic and continuum enables today in many cases, sufficiently accurate prediction of materials properties and behaviour to be achieved and consequently can contribute significantly to the design of new materials and processes. However, prevailing materials modelling paradigms are capable of focusing on limited aspects of the material behaviour explicitly using mainly one single model.

These models need to draw on so called materials relations, e.g., constitutive equations in continuum, interatomic potentials and force fields in atomistic and mesoscopic models, respectively, and pseudopotential or various approximation assumptions in electronic models (e.g., geometrical idealisations) that are either based on results of other models applied separately or on various phenomenological assumptions to complete the description and be able to perform the simulation (see A. de Baas, *What Makes a Material Function? Let Me Compute the Ways. Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology Projects*, 6th ed. European Commision, Directorate-General for Research and Innovation Industrial Technologies, Brussels, 2017).

Tackling the main challenges for increased uptake of materials modelling in industry

In many cases, such materials relations are designed for specific aspects, e.g., describing a liquid phase of a metal, or the structure of a specific defect, and thus affect the whole accuracy of the modelling for cases were processing or application conditions vary significantly, which is usually the norm rather than the exception in materials science and engineering.

Multiscale or in general integrated materials modelling paradigms, such as parameter free models, enable linking and coupling of models so as to either augment different models by enhanced material relations, even on the fly, or provide simultaneous input or description of multiple phenomena at multiple hierarchical time and length scales. This immensely increases the benefits and application of materials modelling to technological cases. In particular, for nano-enable systems, there is a need to describe the nano-scale materials properties (e.g., atomistic structure) using discrete models (electronic, atomistic, or mesoscopic) and the macro-scale (i.e., device level) behaviour using, usually continuum models. This requires developing methods and means to couple and link models efficiently.

Advanced approaches to integrated multiscale materials modelling

Applications of multiscale and integrated materials modelling (i.e., combining several models, possibly on different or even same scales) is severely hampered by two factors.

The first is technical in nature and pertains to the need to develop computational tools and algorithms and implement them in codes that encompass various model descriptions and allow moving information from one model to the other. This is a technical challenge that is traditionally limited to few academic communities.

The second is a scientific one pertaining to the nature of information moved, i.e., to the homogenisation, localisation and schemes known as scale- or more generally, model-bridging paradigms. These are in turn limited by existing knowhow and difficulties of implementation related to the former technical, challenges.

The SimPhoNy project tackles both of these challenges simultaneously in a complimentary and complete manner. It provides novel efficient means to design, develop and implement integrated materials modelling workflows, including multiscaling, efficiently and rapidly even by non-experts in software engineering on the one hand, and it provides explorations into new coupling and linking science on the other hand.

More specifically, the SimPhoNy consortium objective is to address both technical and scientific challenges pertaining to the fundamental questions of linking and coupling of models, namely filtering and loss of

information between models and continuity and reversibility of information across models applied to various scales.

Novel coupling and linking science and Industrial Applications, Apps and Validation

Another objective is to demonstrate the enhancement and impact beyond the state of the art. To this end, the efficiency of the new developed simulation environment specifically for shortening the development process and time to discover novel nano-enabled materials and products is demonstrated through **a proof-of-concept design of novel simulation tools and Apps**, namely applications fulfilling specific purpose, for a cluster of related technologies of significant economic impact for the nano and micro-engineering European market. Specifically, Apps are developed and successfully demonstrated targeting nano-technologies including nano-printing and nano and microfluidics and foam-forming processes (see Figure 4 and Figure 5). Each such App includes development of novel science and complex algorithms for coupling and linking of various models that operate on various scales whose development was facilitated and accelerated by the use of the SimPhoNy environment.

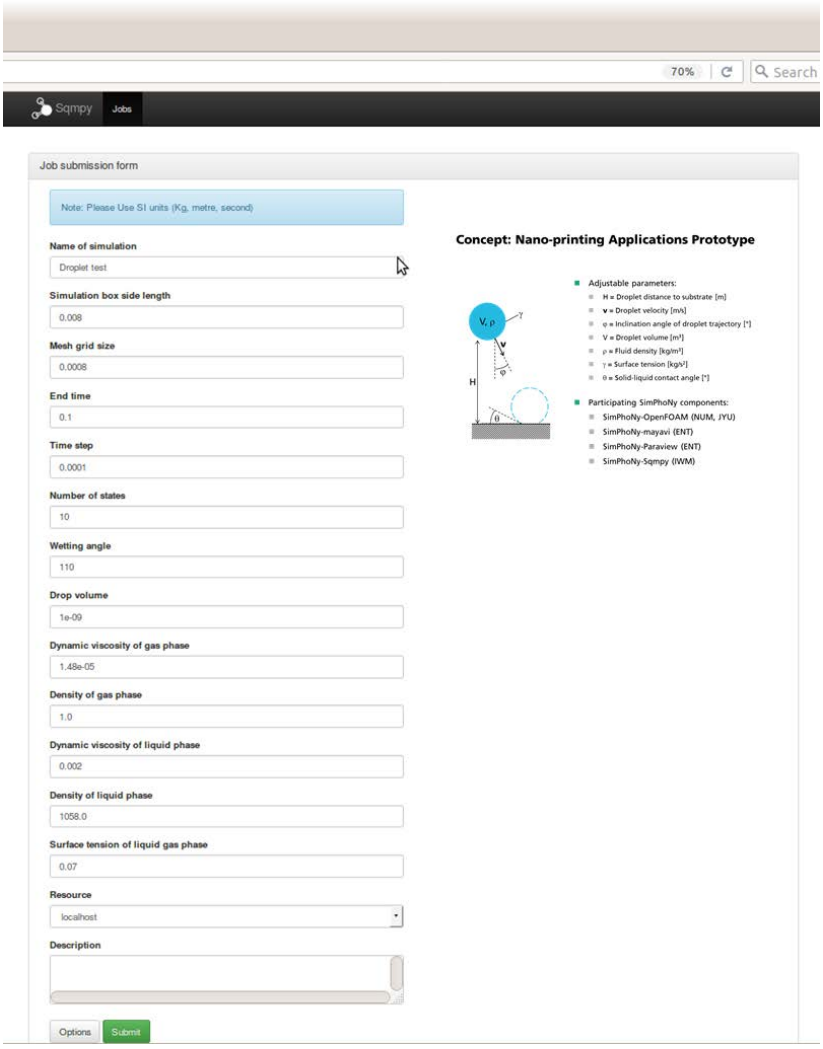


Figure 4: A snapshot of the SimPhoNy web-based user-interface for the nano-printing SimPhoNy App.

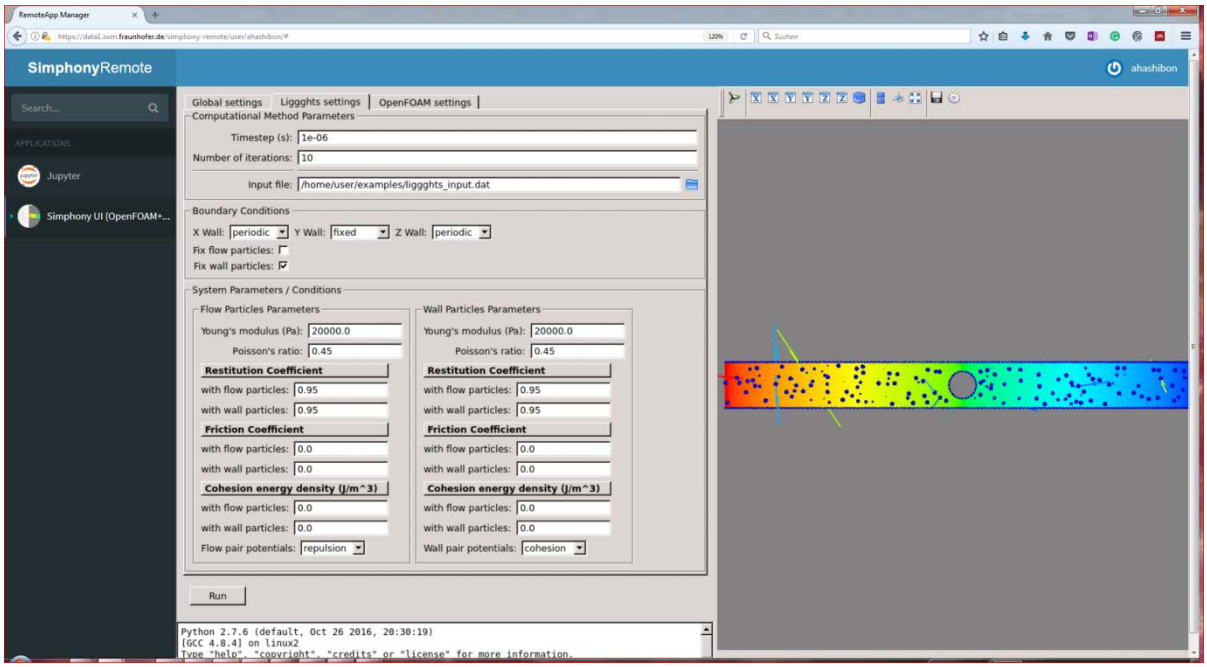


Figure 5: A nano and microfliudic design SimPhoNy App coupling continuum and discrete models on multiple scales.

An Integrated approach based on reusing and extending existing state of the art modelling tools and methods

Accurate modelling of nano-enabled systems requires intricate multi-scale and multi-equation (i.e., multi-physics or multi-model) simulations and integrated workflow approaches that can link and couple (according to the terminology of the EC Review of Materials Modelling) relevant materials behaviour and phenomena on the nano, micro, meso, and macroscales.

Numerous well established simulation tools and models are available for describing a material accurately and efficiently on each of the scales separately. However, advanced applications, especially for nano-enabled systems, required a strongly integrated multi-scale and multi-model simulation framework that allows a seamless and efficient rapid development of linking and coupling of various models each operating possibly on a different scale.

Developing traditional monolithic software tools that incorporate coupling (including concurrent multiscale modelling) of various models is challenging and time consuming, and usually is within the realm of only very few specialized labs and research groups, i.e., out of reach of industries in general and SMEs in particular. Several approaches for linking models, i.e., sequential hierarchical models, applied to various scales are available but have limited applicability to many industrial scenarios.

SimPhoNy takes a different approach as schematically shown in Figure 6, instead of developing own modelling solutions, existing well established and well trusted simulation tools are integrated into a unified framework.

SimPhoNy objective and context is developing an extendable and open platform for the integration of various existing open source and commercial simulation and pre- and post-processing software packages and tools.

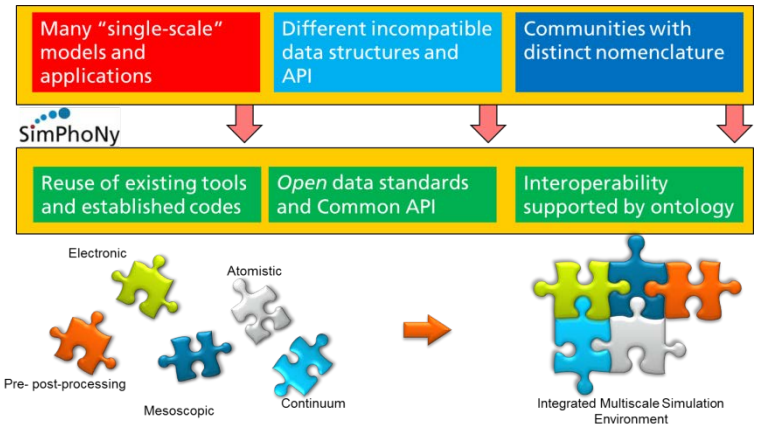


Figure 6: The main approach of SimPhoNy reusing existing well-established simulation tools, augmenting them with data standard interface layers to achieve interoperability and tight integration allowing developed of Integrated Materials Modelling Workflows, including multiscaling.

Standards based approach: Materials Modelling Ontology and Semantic Cross-Domain Interoperability and managing all materials modelling information

To facilitate interoperability between models, i.e., to allow different models, and related tools to exchange information efficiently, a common universal data structures (CUDS) is developed. The CUDS is a metadata schema for representing all information needed to perform a modelling simulation. The CUDS describe all information based on the same vocabulary for all models. To this end, SimPhoNy develops the common universal Basic Attributes (CUBA) which is a constrained list of vocabularies transcending all models. The CUDS contribute to breaking down the language barriers between isolated modelling communities and allows high-level semantic and cross domain interoperability to be achieved, facilitating both data curation, data management, and coupling and linking.

Development of Interoperability Layers: Wrapper Technology

Integration is achieved by wrapping existing simulation packages by an efficient standards based data (CUDS and CUBA) and information interoperability software interface layers designed and implemented in a high level language, namely Python, with a common and minimal application programming interface (API) to the outside world. The SimPhoNy framework allows both linking (sequential execution) and coupling (concurrent execution and tightly coupled equations) of models. Each wrapper can accept CUDS containing all information to perform a model and can execute, i.e., perform the modelling and provide the results to the user.

Covering all models on all scales

The models and corresponding modelling tools integrated cover all models electronic, atomistic, mesoscopic and continuum and allow their application at all relevant scales (see Figure 1 and Table1). The SimPhoNy framework is publically available on http://github.org/simphony under a permissive license allowing its adoption by both proprietary and open source codes.

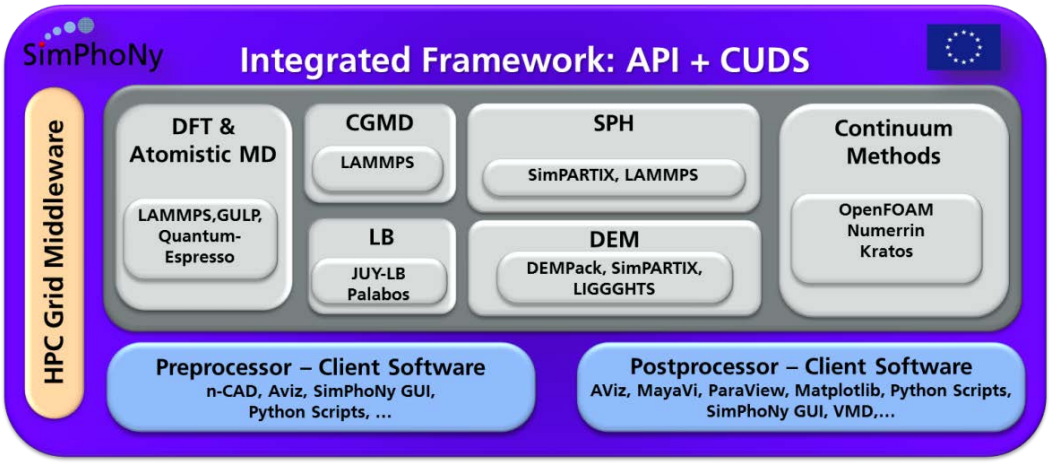


Figure 7: A schematic representation of the integration of various simulation tools into the unified integrated SimPhoNy framework.

Table 1: List of software tools integrated and the type of integration. File-IO uses files to communicate and is a "loose" type of coupling; internal wrapper uses software libraries and is a "tight" coupling of codes.

Application	Method	Model supported	File-IO Wrapper	Internal Wrapper
quantumESPRESSO	DFT	Electronic	✓	
LAMMPS	MD	Atomistic	✓	✓
Kratos	DEM	Mesoscopic		✓
LAMMPS	CGMD	Mesoscopic	✓	✓
LIGGGHTS	DEM	Mesoscopic	✓	✓
SimPARTIX	DEM	Mesoscopic	-	-
JYU-LB	LB	Continuum/ Mesoscopic	✓	✓
Kratos	FEM	Continuum		✓
Numerrin	FEM/FVM	Continuum		✓
OpenFOAM	FVM	Continuum	✓	✓
Palabos	LB	Continuum		✓

Advanced Workflows for coupling and linking

SimPhoNy provides a simple and straightforward to use framework to develop advanced integrated materials modelling workflows. As shown schematically in Figure 8, in step 1, the user prepares a simple python script to create a CUDS data structure containing the complete information needed to start one particular model without reference to the syntactic format of the chosen simulation software tool (i.e., using the SimPhoNy ontology and CUBA, in other words, the SimPhoNy standard semantic "format"). In step 2, the SimPhoNy script adds this CUDS (or send) to a wrapper attached to a specific simulation tool in the backend. The script in step 3 activates the wrapper with a RUN method, which results in performing the modelling simulation using the chosen backend engine (simulation software tool as integrated into SimPhoNy). The wrapper then provides, upon successful completion of the simulation, a new CUDS structure with the results. The user can

then configure the script to extract selected information from the first simulation, perform general arbitrary pre and post processing including homogenisation, localisation, or any other scale or model bridging steps, and create new CUDS for another model. Step 5 and Step 6 are then similar to steps 1 and 2 of the first model, but executed with a new model. Step 4 is the actual coupling and linking step. Depending on the type of algorithms used in step 4, strong coupling, week coupling, or linking can be performed. Linking and coupling of arbitrary models on various scales can then be performed at ease and rapidly.

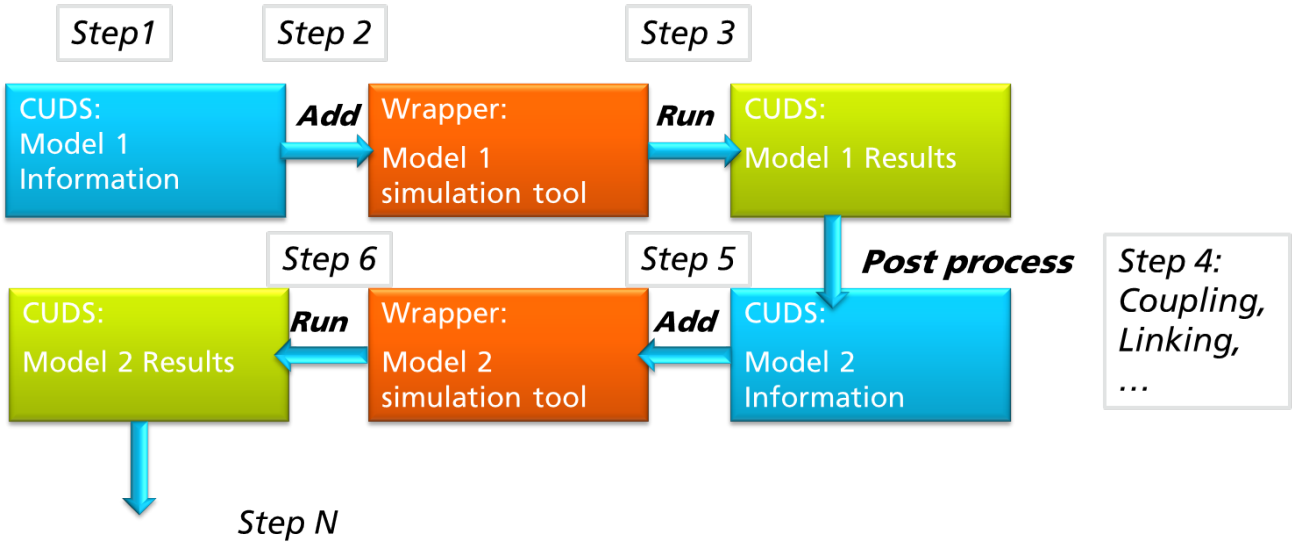


Figure 8: A schematic of a SimPhoNy integrated materials modelling workflow.

A description of the main S&T results/foregrounds

I. A computational simulation framework to couple all models on nano-, micro-, meso-, and macro-scales by integration of open-source and commercial tools into a coherent simulation and modelling environment based on client-server architecture.

SimPhoNy provides an easy to use, extendable and open integrated simulation platform. The platform integrates various open and closed source tools as shown in Figure 3, Figure 1 and Table 1. The underlying interoperability framework based on syntactic, semantic and cross domain interoperability allows seamless integration of the various tools (including simulation as well as pre and post-processing tools) into the framework. This enables the development of intricate multiscale and in general, integrated multiscale materials modelling applications. The main integration is achieved by first wrapping existing state of the art (and novel, in SimPhoNy developed tools) by a software interface layer (wrapper) which translates the syntactic information used by each tool, see Figure 9, to the semantic data structures used in SimPhoNy, i.e., CUDS (see below). Users can then develop python scripts using the generic data structure and information of SimPhoNy to communicate with all models using any of the supported tools, regardless of their formal. The wrappers take care of translating the information from SimPhoNy to the application and back.

An efficient plugin system allows users to custom tailor the SimPhoNy framework as they wish, incorporating only the tools they are interested in. An arbitrary combination of available wrappers can therefore be used to develop sophisticated integrated modelling workflows incorporating any arbitrary collection of models and tools. This constitutes a substantial progress with respect to the state of the art, as no such easy to use tool, supporting rapid development of tools existed. The SimPhoNy core is open source with a permissive, business friendly license and can be downloaded from the project web site.

The simulation software tools incorporated range from quantumESPRESSO for electronic models, LAMMPS, LIGGHTS, KratosDEM for discrete atomistic and mesoscopic models, and Numerrin, OpenFOAM and KratosFEM for continuum models. Additional wrappers to other tools can be developed easily, incuding for closed source commercial tools without access to their codes (using File based wrappers).

The SimPhoNy git hub organisation currently contains **45** repositories (SimphoNy components) reflecting structuring of code and adding new features pertaining to client servers (SimPhoNy-Remote, SimPhoNy-sqmpy) and metadata and ontologies etc. as shown in the list below. Note that all repositories are open source and include documentation and installation instructions.

1. simphony/simphony-framework
2. simphony/simphony-remote
3. simphony/simphony-sqmpy
4. simphony/buildrecipe-lammps_bin
5. simphony/buildrecipes-common
6. simphony/simphony-common
7. simphony/simphony-openfoam
8. simphony/simphony-metaparser
9. simphony/buildrecipe-simphony_ui
10. simphony/buildrecipe-PyFoam
11. simphony/buildrecipe-simphony_mayavi
12. simphony/buildrecipe-simphony_liggghts
13. simphony/buildrecipe-liggghts_bin
14. simphony/buildrecipe-simphony_lammps
15. simphony/buildrecipe-lammps_python

16. simphony/simphony-metatools
17. simphony/simphony-metadata
18. simphony/simphony-network
19. simphony/simphony-liggghts
20. simphony/simphony-kratos
21. simphony/simphony-lammps
22. simphony/tornado-webapi
23. simphony/simphony-ui
24. simphony/simphony-remote-docker-simphony-ui
25. simphony/simphony-remote-docker
26. simphony/simphony-jyulb
27. simphony/JYU-LB
28. simphony/simphony-numerrin
29. simphony/simphony-remote-docker-simphony-paraview
30. simphony/simphony-remote-docker-simphony-mayavi
31. simphony/simphony-mayavi
32. simphony/simphony-remote-docker-scripts
33. simphony/simphony-remote-docker-filemanager
34. simphony/simphony-remote-docker-jupyter-notebook
35. simphony/simphony-remote-docker-base
36. simphony/simphony-metaedit
37. simphony/simphony-paraview
38. simphony/simphony-aviz
39. simphony/traitlet-documenter
40. simphony/simphony-espresso-dft
41. simphony/simphony-nCAD
42. simphony/nfluid
43. simphony/simphony-tools
44. simphony/simphony-palabos
45. simphony/AViz

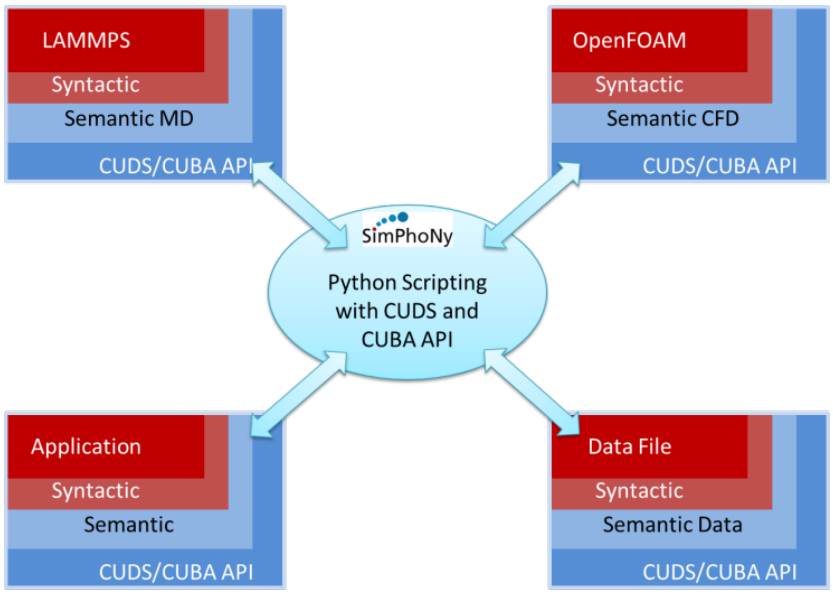


Figure 9: All data and information is exchanged semantically between different software simulation tools and pre/post-processing tools through the CUDS interface.

II. Common interface system for data exchange between methods and scales as well as between pre- and post-processing and simulation tools.

SimPhoNy project exerted substantial efforts to develop common, high-level interoperability layer based on state of the art data and information technology and science. At the heart of the SimPhoNy data interoperability layer is the SimPhoNy Materials Modelling Ontology which covers all models, methods, including elements of pre and post processing. This ontology is available on the SimPhoNy project web site and was within SimPhoNy developed in isolation from recent advances in data science, nevertheless, the basic ontology structure, forming both a semantic network with definitional relations agrees completely with state of the art ontologies, such as the Basic Formal Ontology and will form part of the European Materials Modelling Ontology endorsed by the EMMC.

The ontology defines all entities needed to describe fully the information necessary to perform any computational materials model simulation. It includes on the top level a description of the material system, the boundaries and conditions, the physics equations and materials relations as well as the numerical solver and its parameters, see Figure 10.

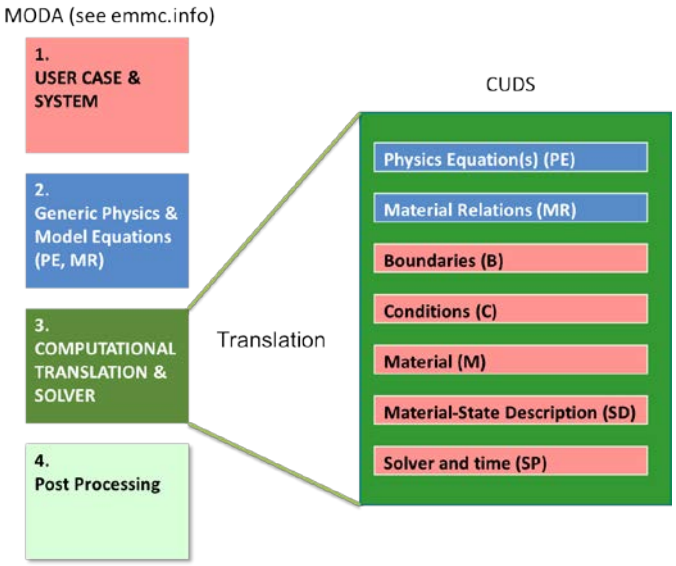


Figure 10: A schematic of the SimPhoNy CUDS containing top-level concepts that map to chapter 3 of the MODA. However an extension of CUDS to include other chapters is straightforward as it requires adding the ontology concepts from the RoMM.

The ontology is used to derive a metadata schema that is used both for serialisation, storing data to files, and defining the CUDS data structures that hold all information.

All wrappers to simulation software tools, pre and post processing tools use the same interface to CUDS. A special method, called a CUDS container allows users to query the information stored in the CUDS, check consistency and completeness, and add, change, delete or iterate over all data entities.

III. Advanced pre and post processing applications

While numerous Computer aided design (CAD) solutions are available for large scale systems (CFD and FEM tools), a similar easy-to-use powerful and feature-rich equivalent to atomistic and particle systems does not yet exist. To fill this gap, In SimPhoNy both existing and new pre- and post-processing solutions are developed, enhanced and integrated within the simulation environment.

Work is performed on four different pre/post-processing and visualization solutions. This includes the AViz visualization package, development of a completely new open source system for pre-processing of particle and mesh based fluid simulations and two VTK based tools, namely simphony-mayavi and simphony-paraview.

In addition, a User Interface component for developing applications (SimPhoNy-UI) and a web-based interface (SimPhoNy-Remote, SimPhoNy-sqmpy) for managing job submission and application development in a client-server setting was developed.

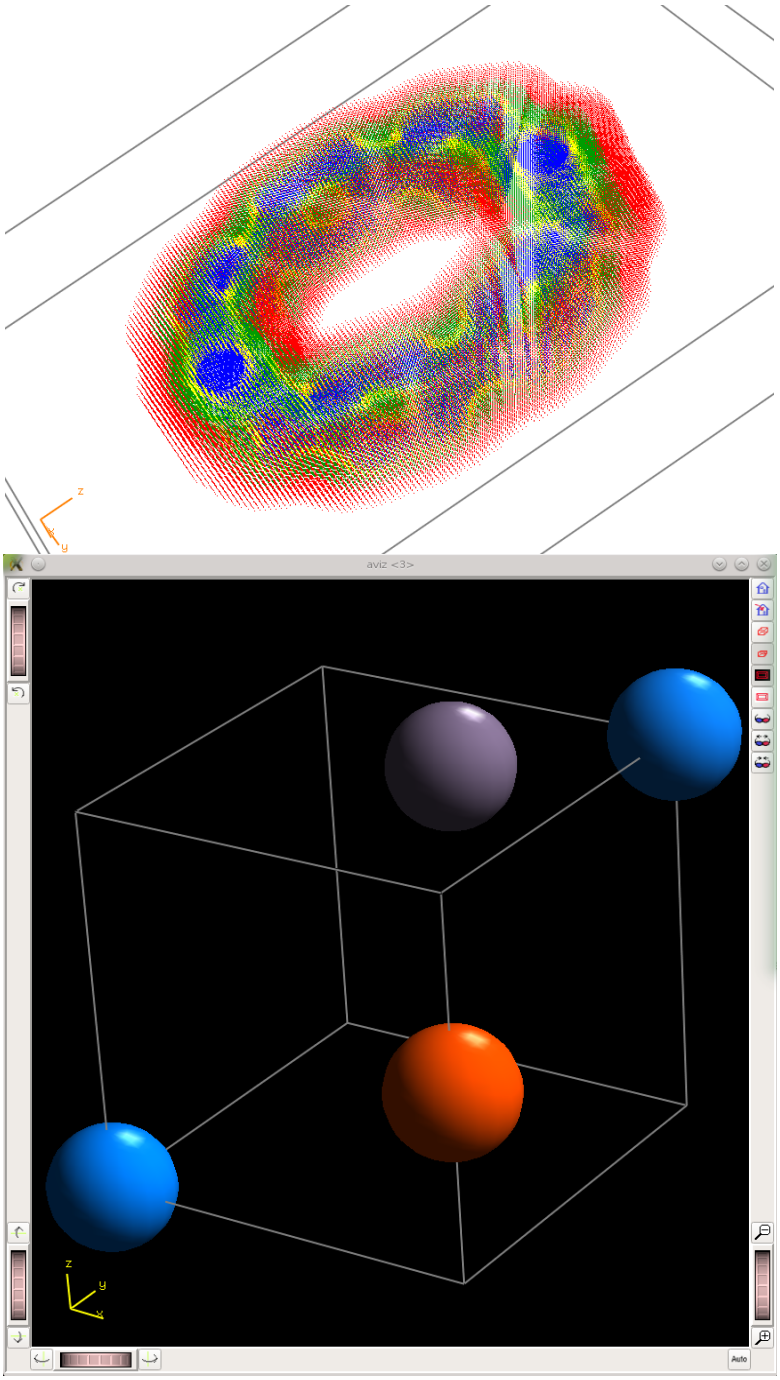


Figure 11: Example of electronic density visualization using dots in AViz (top) and a snapshot of an AViz instance showing a simple system where each atom/particle has different colour (bottom).

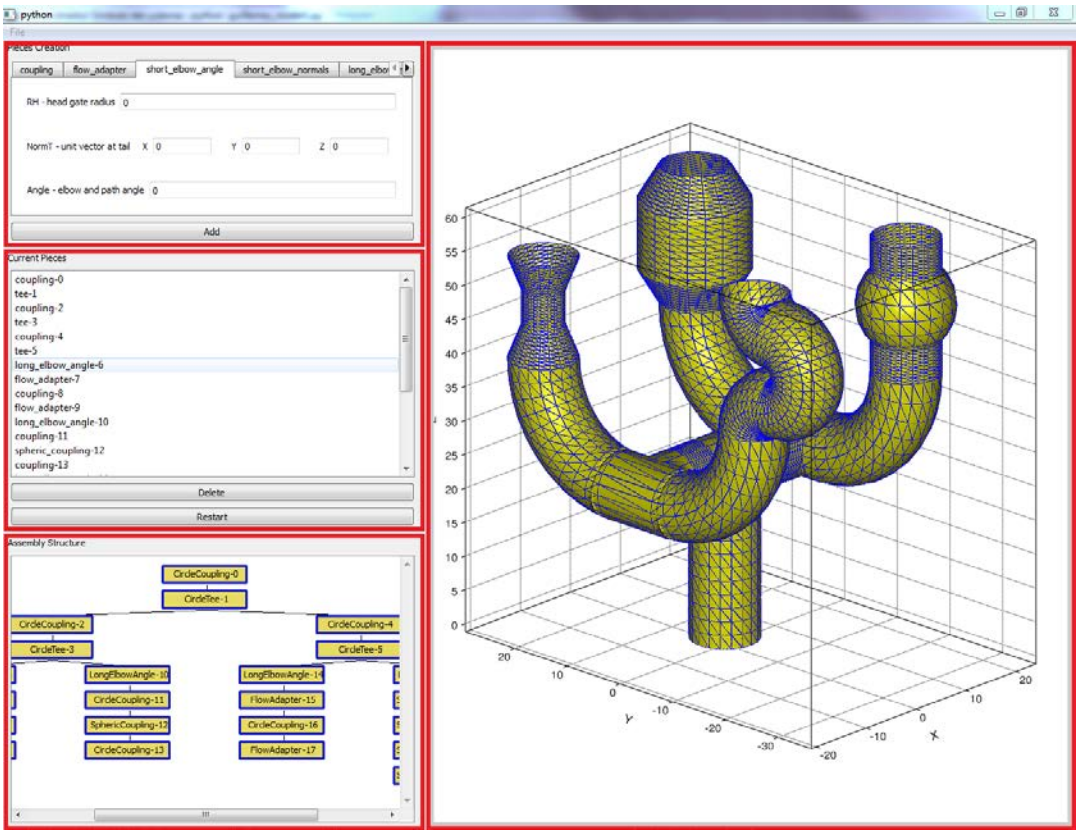


Figure 12: Screenshot of the GUI main window of NCAD-Fluid, a CAD like system for mesoscopic modelling.

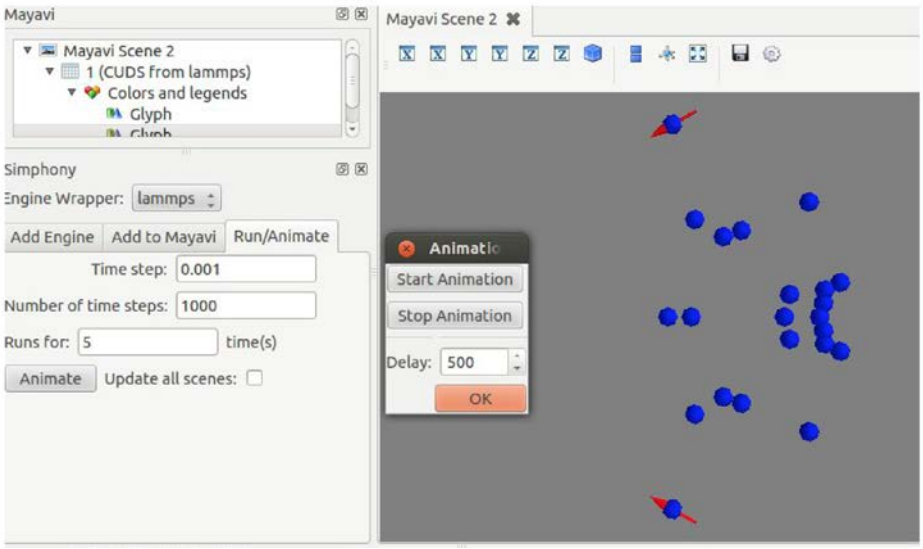


Figure 13: Example of Integration of SimPhoNy and Mayavi. Running an engine wrapper and updating the visualisation using the "Run/Animate" tab in the GUI. In this screenshot, a LAMMPS engine wrapper named "lammps" is added to the GUI and is selected. As the user presses the "Animate" button, the engine wrapper is run for five times and at the end of each run, the visualization is updated using the updated data from the engine wrapper.

IV. Native SimPhoNy client-server solutions with GUI tools.

SimPhoNy developed a set of tools allowing users and developers to deploy SimPhoNy on a server side and access it through multiple client tools. Three options are provided, two of which are operational with graphical user interfaces, namely SimPhoNy-Remote and SimPhoNy-Sqmpy, and one, SimPhoNy-Network, is currently developed on the specification level providing command line and scripting API for future extensions of SimPhoNy. SimPhoNy-Remote brings the application to the data and provides the user with a thin client to control and visualise the application using a web-browser. State of the art virtualisation and remote access are employed allowing control of SimPhoNy applications even from tablets and smartphones. SimPhoNy-Sqmpy, is a job submission and management system allowing users to submit batch jobs to remote servers and monitor the execution. It also allows users to fetch the data for additional processing. An extension to SimPhoNy-Sqmpy allows creating custom user interfaces in a web-browser enabling users to customise the application and then submit it. SimPhoNy-Network is a command line interface and basic API allowing execution of remote components. It is developed specifically for future implementations that rely on distributed computing; hence it allows SimPhoNy to be network aware. In addition a Job Description file is developed that can be integrated into SimPhoNy-Sqmpy or SimPhoNy-Remote to save the status of the job.

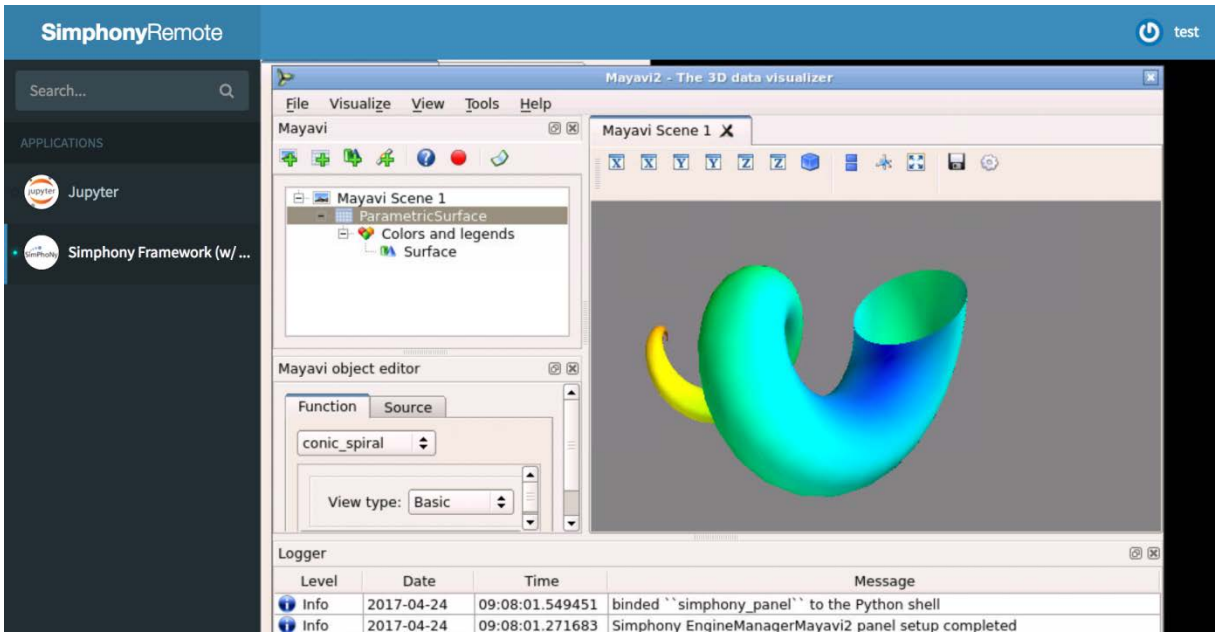


Figure 14: A second screenshot of SimPhoNy-Remote showing a heavy visualisation running inside a web-browser.

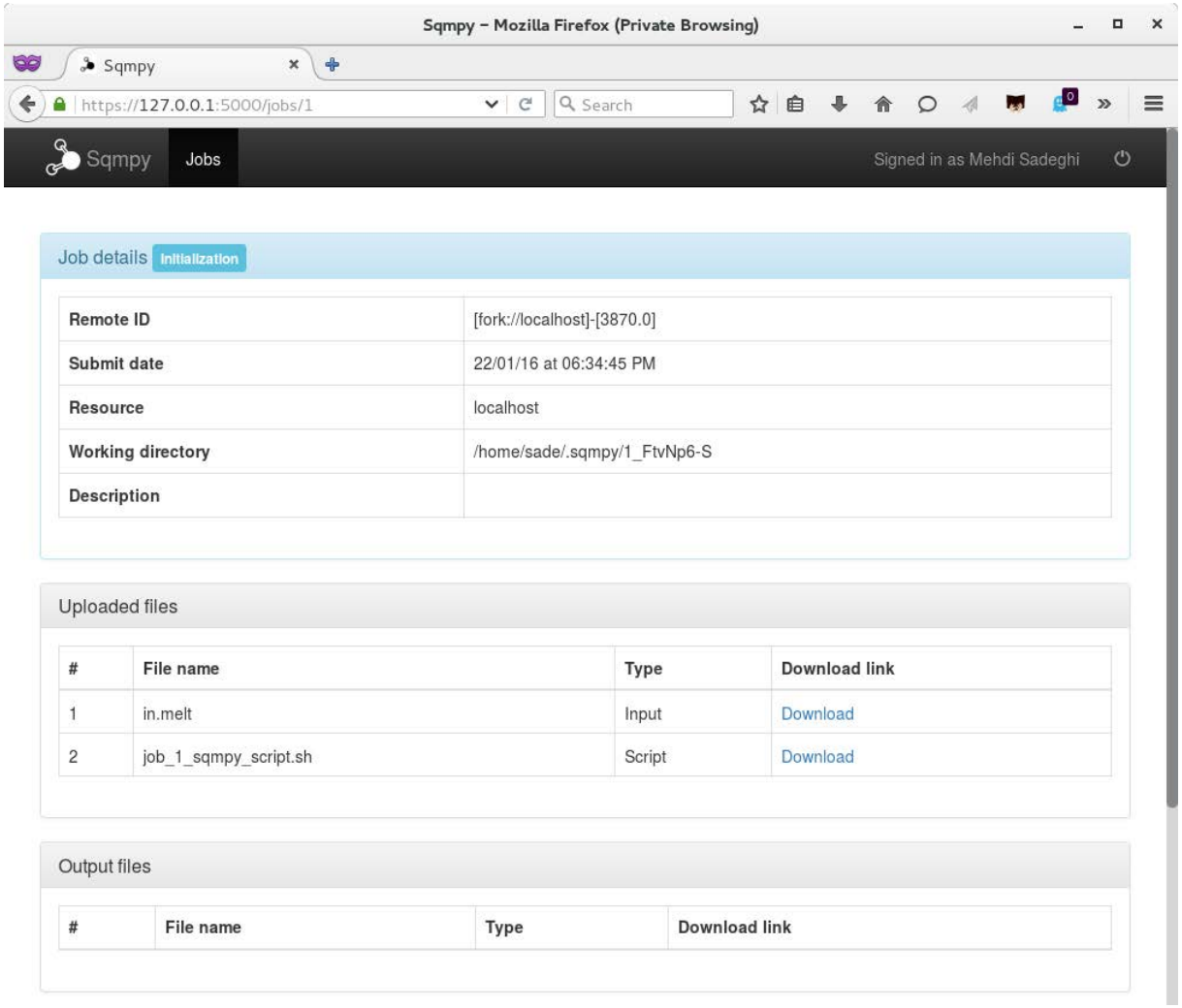


Figure 15: The information web-page of SimPhoNy-Sqmpy displaying the status of a job. The user can access this information from any web-browser

V. Ensuring the interoperability of simulation tools by combining efforts with other projects, at the same time, further develop and comply with industry and research standards.

The third main result of SimPhoNy is the intensive interaction with cluster projects (cluster 5+1 and the ICMEg CSA), and especially with the European Materials Modelling Council (EMMC) to develop all encompassing, reference standard for interoperability. In particular, while the ontology, and CUDS was developed in isolation from recent advances in data science, nevertheless, the basic ontology structure, forming both a semantic network with definitional relations agrees completely with state of the art ontologies, such as the Basic Formal Ontology and will form part of the European Materials Modelling Ontology endorsed by the EMMC.

VI. Demonstrating the efficiency of the modelling framework in a relevant nanotechnology field by design and development of specialized multiscale modelling tools that can reduce the time to discover novel nano- and micro-fluidic devices for biomedical, chemical and energy related applications.

The final major result of SimPhoNy is the development of advanced multiscale and integrated materials modelling workflows based on the SimPhoNy framework. SimPhoNy focuses on a cluster of related technologies of significant economic impact for the nano- and micro-engineering European market. Specifically, we consider four practical problems, two of which affect bio-medical and health applications, namely design of microfluidic systems for medical diagnosis and NEMS devices for detection of molecules, and two which affects other nano-technologies, namely nano-printing and coating, for e.g. production of microarrays and printing of nanoparticle inks, and foam-forming processes.

Substantial developments to the state of the art of coupling and linking including scenarios that cover all main multi-scale and multi-equation modelling, including

1. Sequential hierarchical multi-scale modelling, i.e., linking according to the RoMM
2. A heterogeneous multi-scale method (HMM) whereby macroscopic properties in continuum models are obtained on the fly from discrete model simulations. These fall into the iterative modelling in the language of the RoMM
3. Concurrent multi-scale materials modelling workflows, which also falls under the category of concurrent coupling of MD and CFD
4. Covering coupling and linking of same and multiple different (including vastly different) time and length scales

Advancements included both elements of new methodologies based on the framework as well as new science for the coupling and linking. The various application domains tackled are shown in the table below.

Coupled Scales/Models	Applications & Design Tools
DFT-MD: Nano-Micro (e/a)	NEMS
(CG)MD-PD-CFD: Nano-Micro-Meso (a/m/c)	Nanocolloids, Nanoprinting
PD-CFD: Nano-Meso-Macro (a/m/c)	Foam forming processes, fibers, nanocellulose suspensions
MD-CFD: Nano-Meso (a/m/c)	Flow in nano/microfluidics, removing gas bubbles

(1) A model for coupling the nano-micro scales is developed and used to calculate the frequency response of a nanotube as a function of mass of the additional atoms in the nanotube.

Electronic structure calculations based on density-functional theory (DFT) are linked to atomistic molecular dynamics simulations using the interface libraries developed. 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 was on development of a transfer protocol between the different models and 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.

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 was then shifted to WP5 where an application based on this coupling for calibrating NEMS devices was developed (IIT).

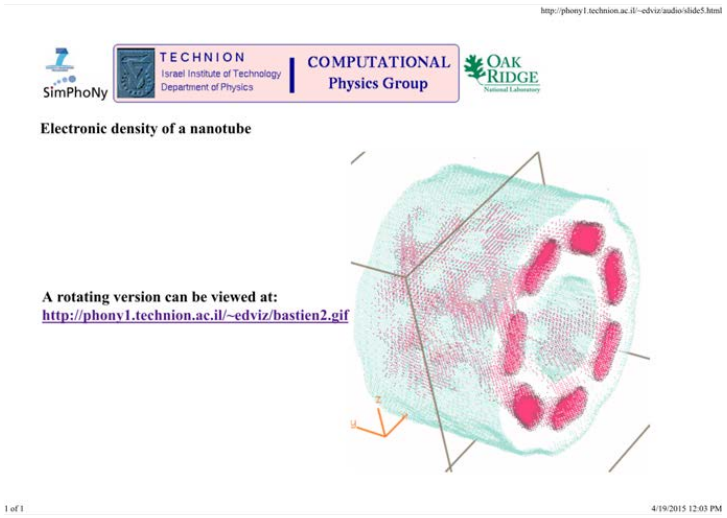


Figure 16: Electron density visualization as part of the linking (using AViz)

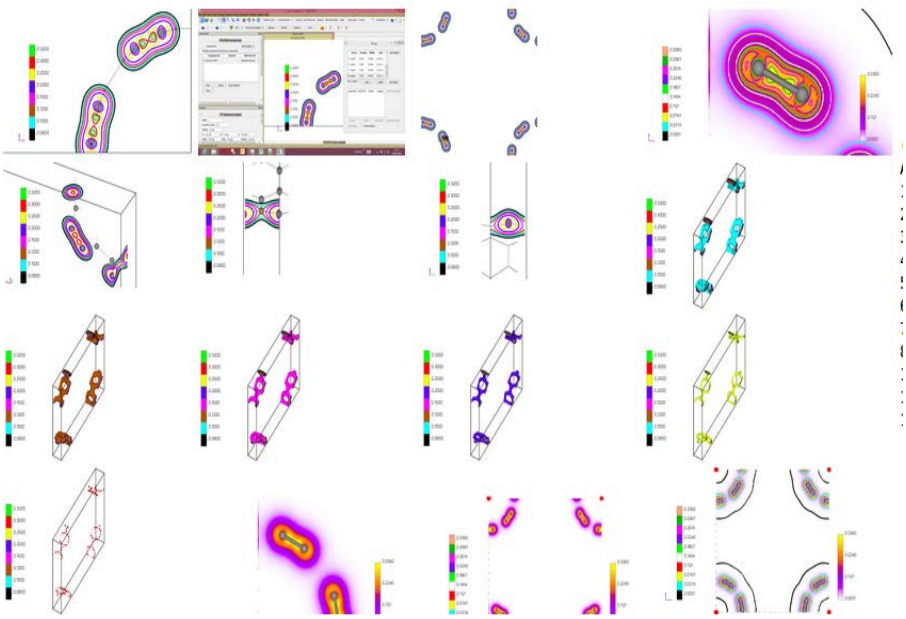


Figure 17: Examples of electron density visualizations as part of the MD-DFT workflow done by n-CAD

(2) A model for nano-micro-meso scales coupling in nano/microfluidic systems is developed and implemented.

The goal is to create a multi-scale simulation tool for modelling the transport of nano-colloids and particles suspended in a multicomponent (i.e. multiphase) fluid in complex confinement in the presence possibly of an external electromagnetic field and internal electromagnetic interactions. The nature of the problem requires applying continuum and discrete models at nano, micro, meso and naturally the macro (device level) scales. Different modelling and coupling and linking approaches are developed in SimPhoNy beyond the state of the art. Models include tightly coupled equations to describe a multiphase fluid in the presence of particles using two separate modelling approaches both of which are based on diffuse interface models but that differ in the way they describe the phases and the interfaces. Multiple discrete models for the particle (colloid) phase are considered, ranging from point like particles, collection of point-like particles, and solid (mesoscopic) particles. The model included a fluctuation SPH model coupled with coarse grained MD (IWM), a fluctuation lattice Boltzmann model coupled with coarse grained MD (JYU) and a drying model in SPH (IWM). This model will enable simulations of wetting and spreading of nano-colloidal particles (JYU and IWM).

Iterative coupling (see https://emmc.info for the terminology) are developed to couple the (tightly coupled) continuum CFD models with the discrete particle models. The iterative coupling is essentially a concurrent multi-scale modelling, whereby both models are solved at each time step. Hydrodynamic fluctuations of the particles are incorporated as well as drying. Methods based on Lattice-Boltzmann and Finite Volume approaches are coupled to CGMD and DEM.

While SPH was used initially in the project, recent advances dictated that using FV methods are more efficient, and focus on them was made instead. Additionally, focus was on testing the best models that are of significant to future applications in industry and in particular for the prototype applications in WP5.

The coupling and linking has been implemented both in SimPhoNy and as stand-alone (syntactic) tools to verify the SimPhoNy models. Comparison to experiments has been conducted. The problems

tackled proved to be challenging as they required developing coupling and linking schemes beyond the state of the art, hence focus in SimPhoNy was to validate against simple cases.

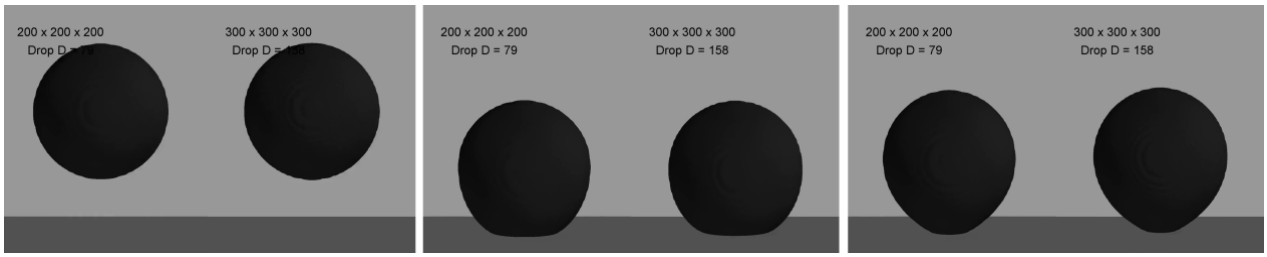


Figure 18: Three snapshots of two dynamically similar drop impact simulations. The drop diameter in the right drop is two-fold compared to the left one, i.e. lattice spacing in the right simulation is halved.

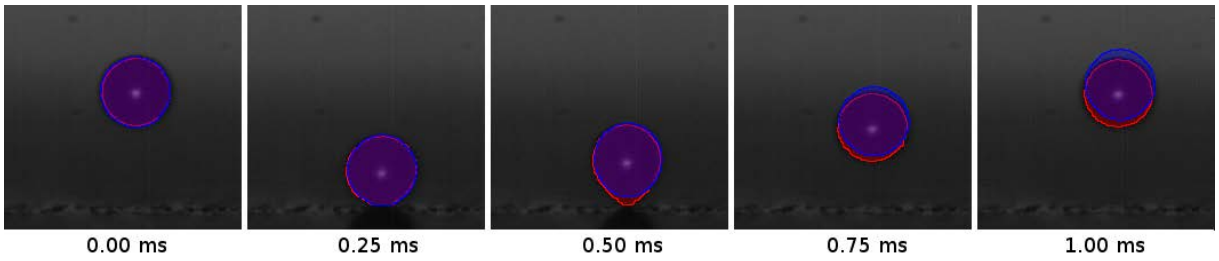


Figure 19: Comparison of five experimental and simulated video frames. Red and blue colours indicate simulation and experiment, respectively.

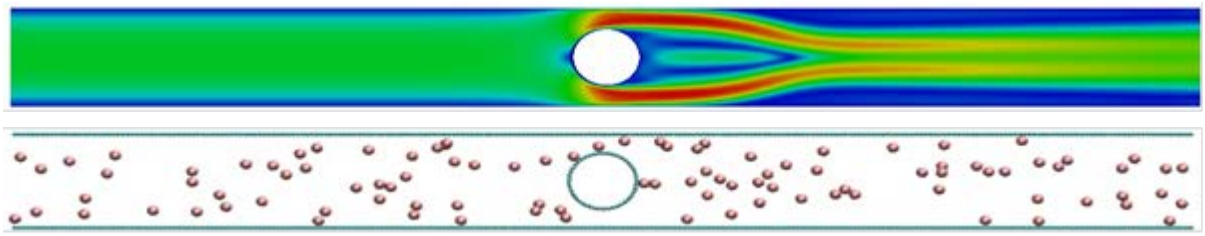


Figure 20: A demonstration of the DEM-CFD coupling for the flow in a channel with a circular obstacle in the middle.

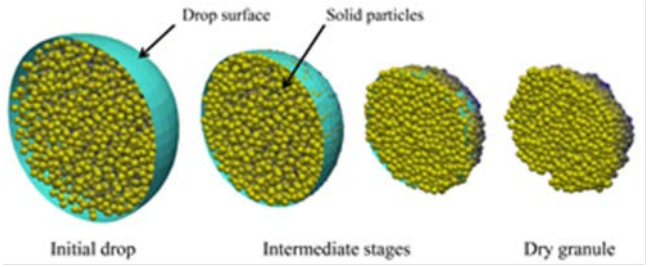


Figure 21: Drying of a free floating drop using CFD-CGMD (utilising DEM-FVM) coupling (IWM).

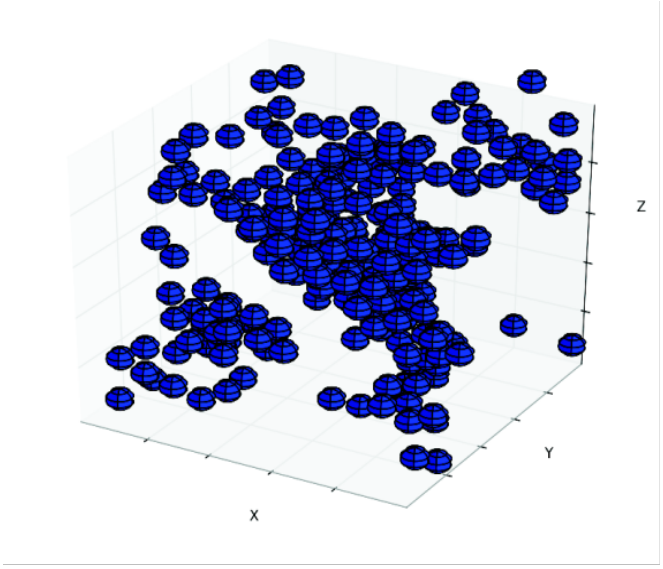


Figure 22: Clustering of nano colloids in a small flow channel. The fluid is simulated with LBM, and the suspended colloids are modelled as point-like particles and their interactions are described by the DLVO theory. The clustering is due to short-range attractive interactions between electrically-charged colloids.

(3) Nano-fiber and foam suspensions using three models: CGMD-Particle DynamicsD (DEM) -CFD.

A novel approach consisting of macroscale continuum hydrodynamic model supplemented with mesoscale model to resolve the macroscale stress tensor (constitutive equation) is introduced. To test the coupling procedure a 1+1 dimensional macroscale Poiseuille flow simulation was chosen at which the macroscale stress tensor was computed from the mesoscale system. In this test a simple power-law Generalized Non-Newtonian Fluid (GNF) model was used. In another test a real mesoscopic foam model (DySMaL) was used. To extend the coupling to multiphase bubble flows the coupling ability (stress, strain and relative velocity coupling) to mixture-model was built to SimPhony framework. This implementation was tested and validated against Dahl's (Dahl, 1993) settling example. To deal particulate flow near walls a new shear dependant boundary condition was implemented and validated using glass pipe experimental data (Jäsberg;Selenius;& Koponen, 2015) for aqueous foams (also fibre-laden). Furthermore the ability to model flexible fibres was implemented to Kratos DEM engine. There has been also working going on to couple DySMaL with Numerrin engine to further extend the validation of the coupling procedure, the design of the coupling between a macroscopic description of a complex rheological fluid, and a mesoscopic model describing the detailed dynamics of the fluid; the mesoscopic model is itself a coupling between DEM particles (bubbles and microfibers) and a fluid (JYU, NUM, CIM/QNT) and the design of coupling algorithm and design of mixture model implementation to wrappers (NUM).

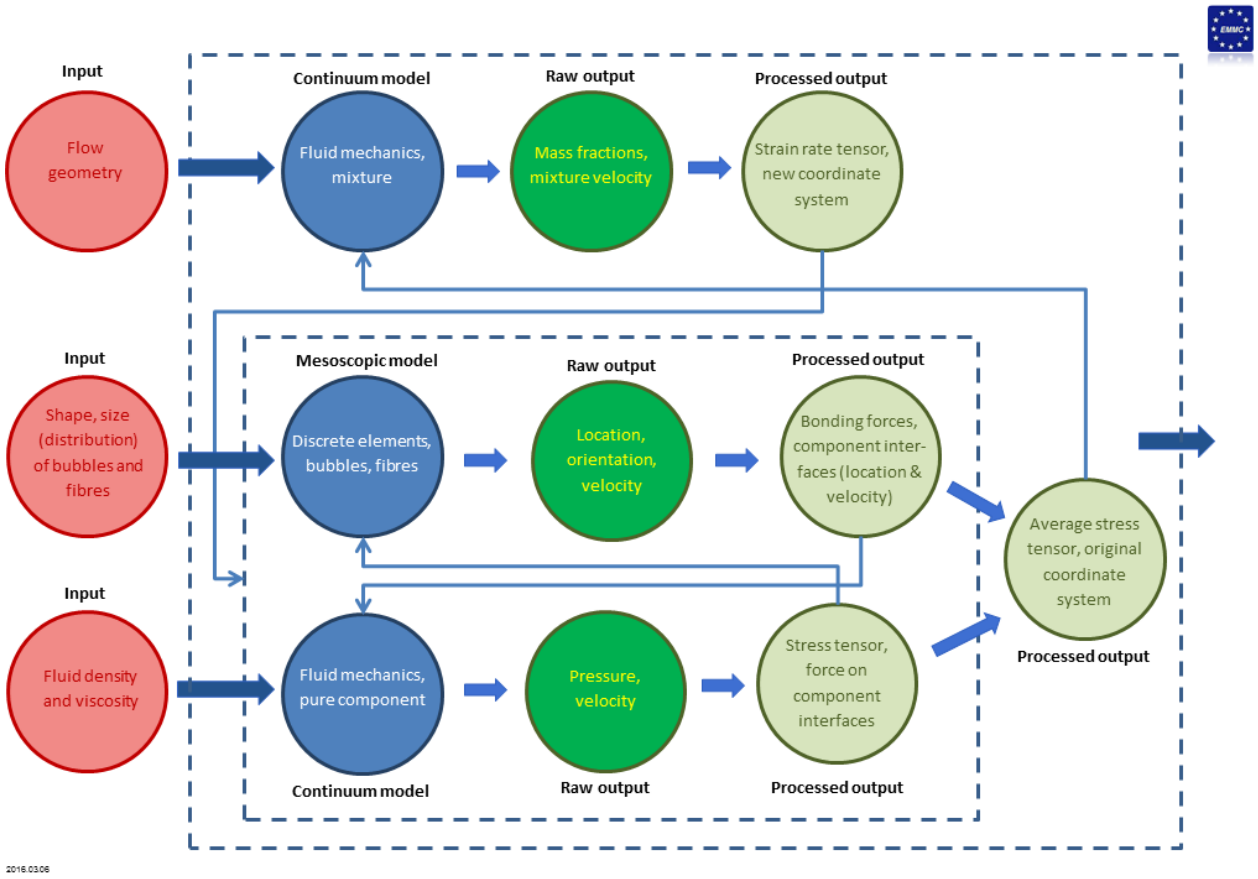


Figure 23: Model workflow for the Case 1 in Task 4.3, i.e. fibres in micrometer scale or above (MODA workflow template by EMMC for loosely coupled models

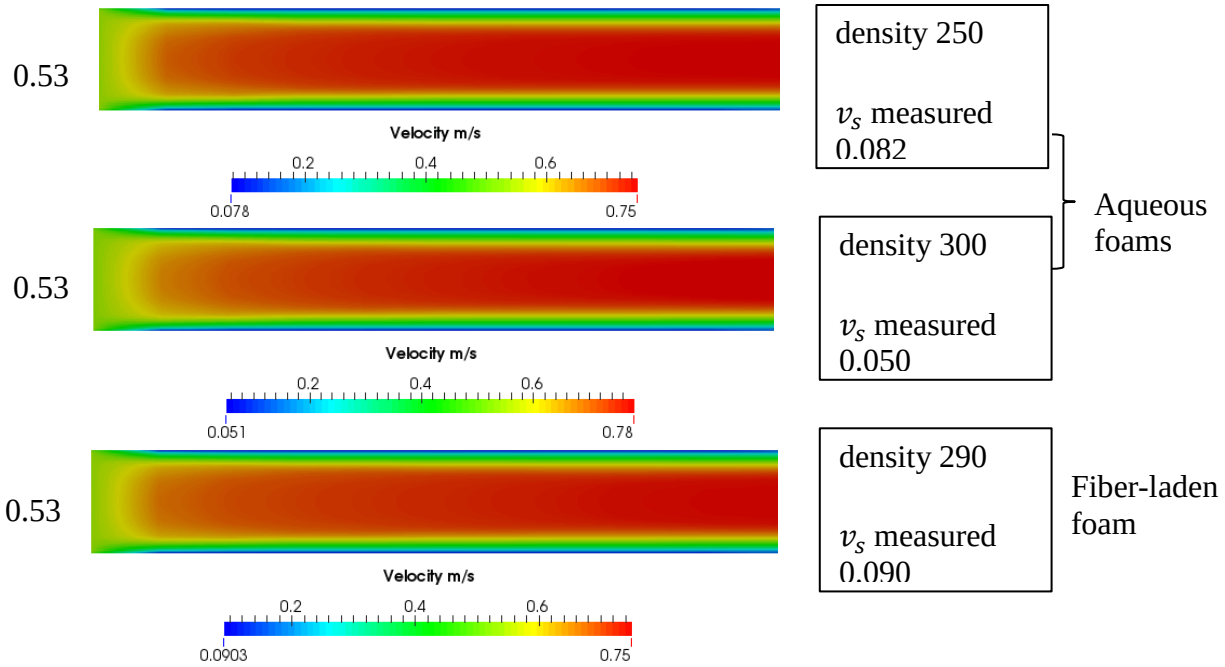


Figure 24: Computed and measured slip velocity comparison for different aqueous foams

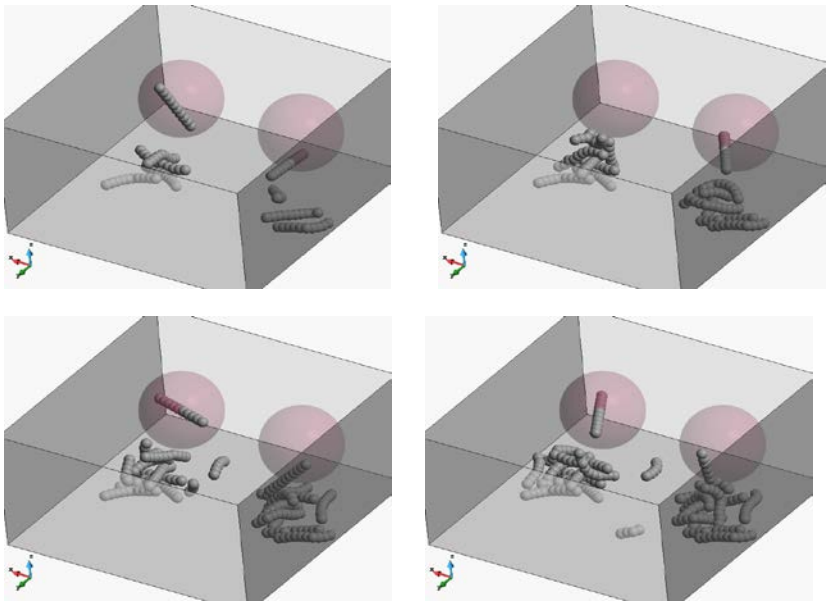


Figure 25: Snapshots of a computation of breakable fibres.

(4) Nano-meso coupling model: A nano-meso coupling model is developed using MD-CFD for modeling of nano/microfluidic systems.

The goal is to develop a "nano-meso scales" coupling of atomistic Molecular Dynamic (MD) and continuum Computational Fluid Dynamic (CFD) models supported in SimPhoNy for modelling nano/microfluidic systems. The need for such a heterogeneous multiscale method (HMM) arises from the fact that in contrast to the macroscopic treatment, the no-slip boundary condition does not always hold in nano-fluidic systems and the assumptions of the continuum (CFD) approximations become inadequate at the solid-liquid interface. Therefore, the coupled CFD-MD approach provides a powerful instrument as a remedy to this drawback, where a natural description of the slip behaviour at the boundary is included in this procedure by representing the liquid flow in vicinity of the boundary using atomistic models. This will also enable a systematic understanding and quantification of the role and extent of the slip in real-world engineering systems.

For the present problem, the fluid was modelled at the macro scale by the CFD SimPhoNy modelling engine wrapper based on OpenFOAM® and at the atomistic level by the MD SimPhoNy engine wrapper based on LAMMPS. The rheological properties of the MD fluid are calibrated to match the respective values of the macroscopic fluid phase. A straight channel with Poiseuille flow velocity profile has been used as the model system. SimPhoNy was applied for running and orchestrating the individual simulations through the wrappers and for realizing the coupling between both scales by transferring the requested data from CFD to MD and vice versa. Here, the calculation of the velocity fields is achieved within the SimPhoNy environment by extracting the relevant data from the individual engines or simulation components.

For the validation of the applicability of the concurrent multiscale modelling using an MD-CFD (weak) coupling approaches (see https://emmc.info/moda-workflow-templates), a reference system was additionally chosen that was small enough to model completely by MD and large enough to be modelled by CFD separately (i.e., an all atomistic and all continuum simulations on the same system under same conditions). Comparing the results thus obtained from both systems without coupling to

those obtained with coupling on the same system provide a direct validation of the coupling schemes used and of the SimPhoNy wrappers.

The methods and models were additionally applied to study complex nano-fluidic systems, in which the surface of the channels are structured on the nano- or micro-scales and the effect of these features on the flow behaviour was investigated. Moreover, a variation of coupling and simulation parameters shows the scope of adaptability of the SimPhoNy framework on this problem.

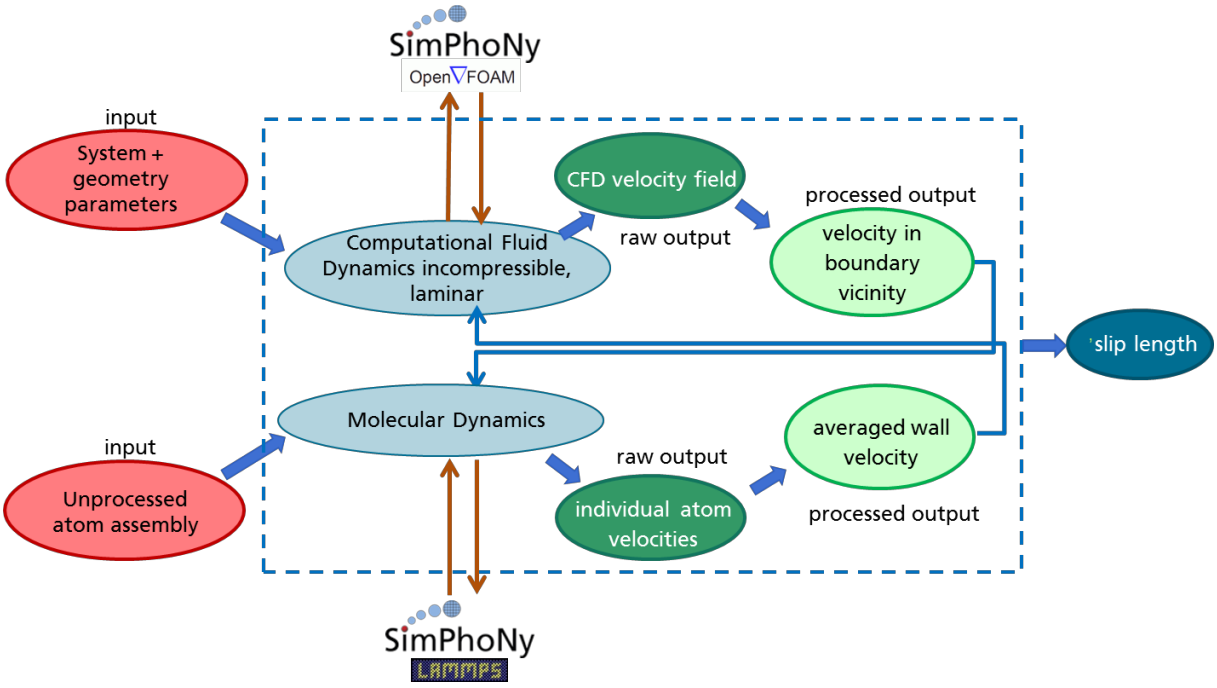


Figure 26: Flow chart of the CFD-MD coupling procedure using the Lammps and OpenFOAM wrappers from the SimPhoNy environment.

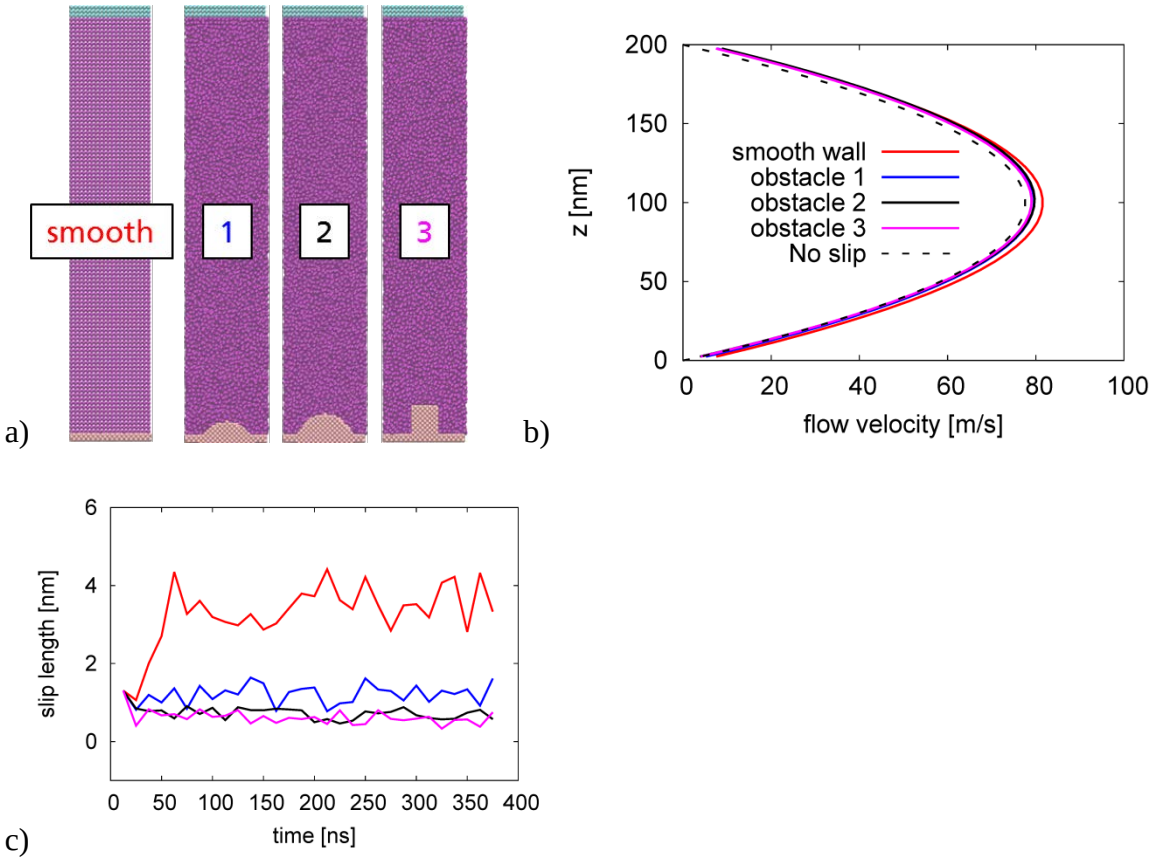


Figure 27: Sample overview (a), CFD flow velocity profiles (b) and temporal evolution of slip length (c) for simulations with different roughness at the atomistic solid wall.

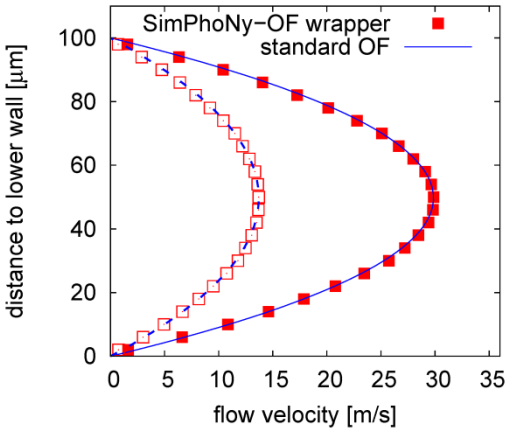


Figure 28: Comparison of velocity profiles of Poiseuille micro-channel flow gained by standard OpenFoam and pure SimPhoNy-OpenFoam wrapper tool showing same results therefore validating the operation of the SimPhoNy wrappers.

Highlights of most significant results

- Novel heterogeneous multiscale materials modelling for foam forming processes and nano-fluidic channels
- New Discrete-Continuum coupling for particle flow and nano-printing applications
- Novel mesoscopic models for coupling particles and fluids dynamics by means of massless particles
- Slip boundary conditions and constitutive relations obtained on the fly by multiscale materials modelling of particle-continuum

(5) Nano-technology applications and validation

The focus is on a cluster of related technologies of significant economic impact for the nano- and micro-engineering European market. Specifically, we consider four practical problems, two of which affect bio-medical and health applications, namely design of microfluidic systems for medical diagnosis and NEMS devices for detection of molecules, and two which affects other nano-technologies, namely nano-printing and coating, for e.g. production of microarrays and printing of nanoparticle inks, and foam-forming processes.

VII. Nano-printing experimental data and validation

Nano-printing experiments are used for the validation of the nano-printing application. Experiments include characterization of droplet size, shape, and morphology of solid ingredients

In a first instance, experiments were conducted for 70 µm as well as 500 µm diameter droplets of deionized water and glycerol solutions as liquids impinging on hydrophilic, hydrophobic as well as superhydrophobic surfaces. After initial simulations for validation which exhibited good agreement between simulation and experiment, the boundary conditions were refined and an additional series of experiments was conducted, this time focusing on ~70 µm, 140 µm and 210 µm droplet diameters as well as hydrophobic and superhydrophobic surfaces. The experiments further featured deionized water, 25 wt% Glycerol and 50 wt% Glycerol as samples as well as two droplet velocities. Consequently, a database of experimental cases was created exhibiting different Reynolds (Re) and Weber (We) numbers. Additionally, software for post-processing of high-speed experimental images was created and optimized. Finally, experiments for the high-speed visualization of beads in droplets were conducted (see figures below).

Based on the work conducted for this deliverable, a database of experimental cases for the simulation validation has been created. Droplet spreading, rebounding and bouncing, depending on the surface properties, was recorded for various combinations of droplet diameters, velocity and viscosity and consequently different Re and We numbers. Additionally, a case for droplet sticking on superhydrophobic surfaces was discovered which could be investigated further. First results for beads in droplets were generated and improved results are expected when combining a flash source for side illumination which could be realized in future experiments.

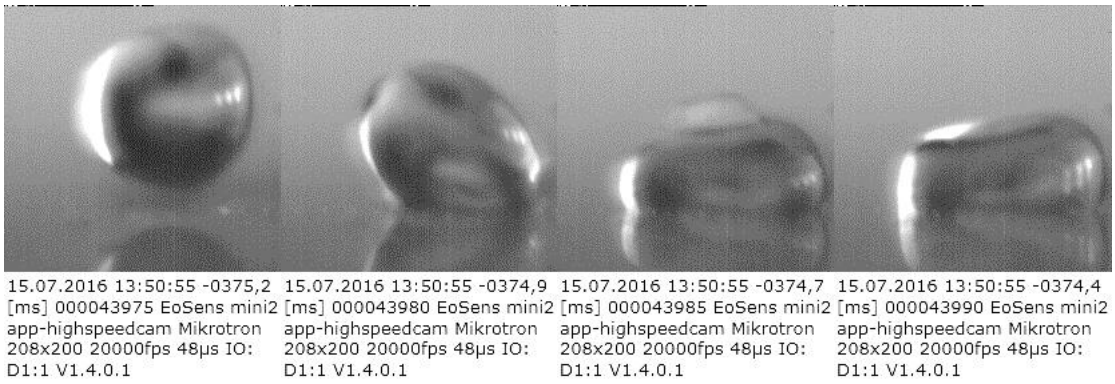


Figure 29: Image series of a ~ 500 µm water droplet containing a single polymer bead comprising magnetic particles for better contrast impinging on a hydrophobic surface.

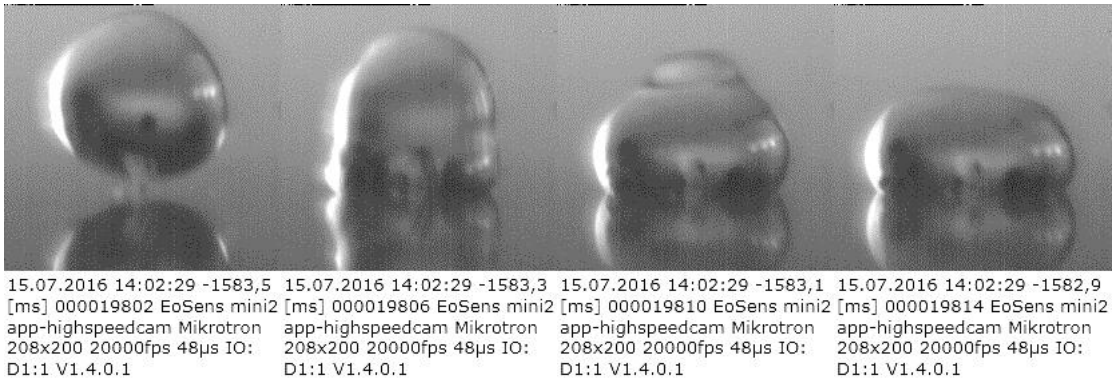


Figure 30: Image series of a ~ 500 µm water droplet containing a number of polymer beads comprising magnetic particles impinging on a hydrophobic surface

VIII. Nano-printing application: Design tool for nano-printing of colloidal particle applications

Based on the developments of multi-scale modeling of nano/microfluidic systems and nano-colloidal droplets, a proto type application is developed for the simulation of nano-printing processes (IWM, ENT, JYU, NUM). The specifications of the application are derived and are determined during the project. The nano-printing application is entirely developed on top of the SimPhoNy framework using the OpenFOAM interface wrapper, i.e., based on a continuum CFD model. Extension to include particles and colloids is straightforward but will result in long execution times that will make it hard for the industry partners to evaluate in a timely manner, hence in this deliverable focus was given to fast execution codes (from few minutes to some hours). Integration of discrete models has been demonstrated and validated.

An application based on SimPhoNy-Sqmpy is developed. A customized web-based user interface is developed on top of Sqmpy that accepts physics based properties and parameters to allow industry end-users to define the user case without the need for technical knowledge on the methods or even the models employed. Sqmpy then creates a custom SimPhoNy script, and submits it for execution. The user receives feedback on the

execution and can then download the results for further post-processing using e.g., SimPhoNy-Paraview or SimPhoNy-Mayavi. The application demonstrated here while simple is already useful for practical nano printing applications. Extension to more complex models including coupling and linking is straightforward and topic for future exploitation.

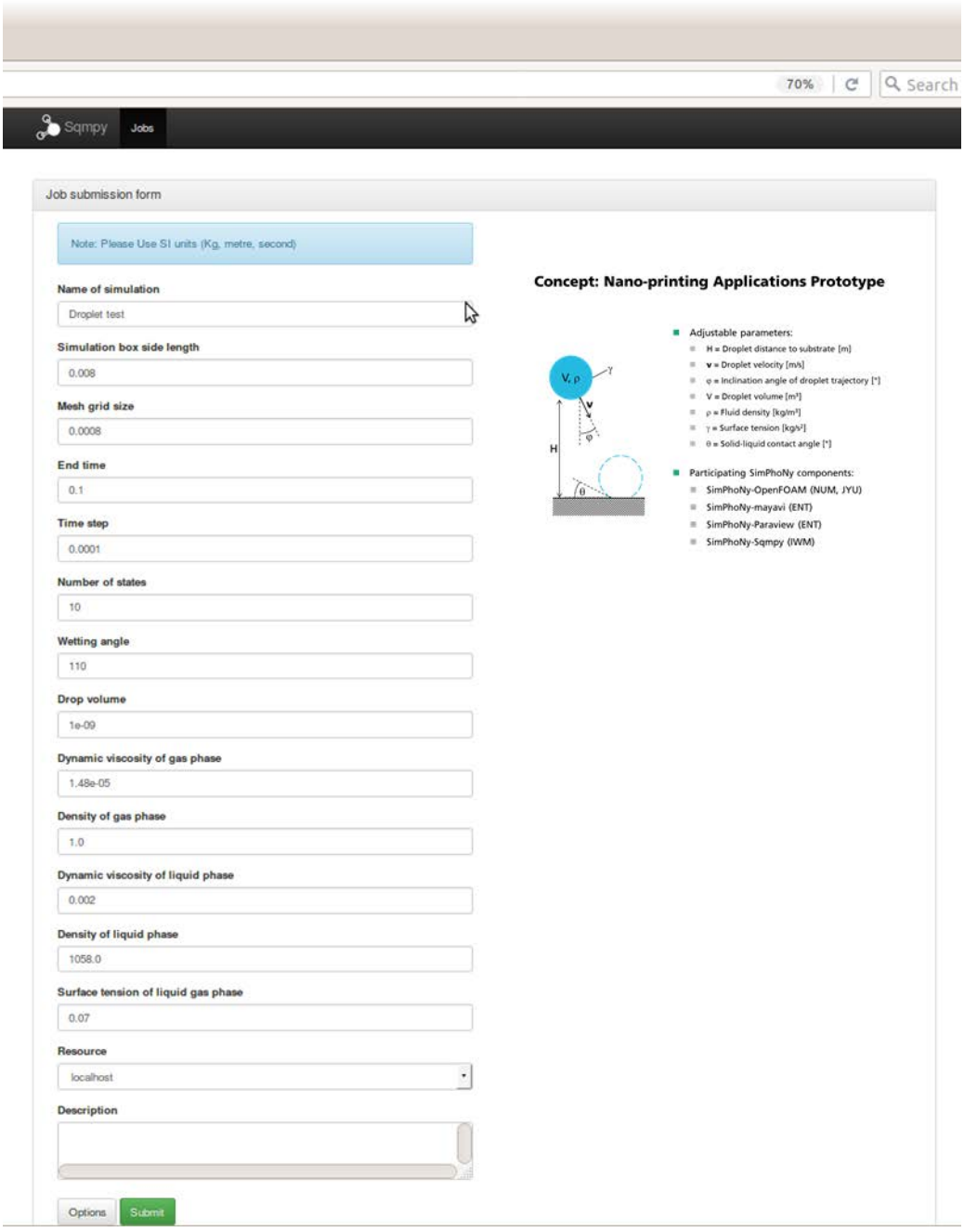


Figure 31: The input interface of the SimPhoNy Nano-printing app shown in a web-browser. (Note: the image on the right is overplayed on the Figure for clarity.

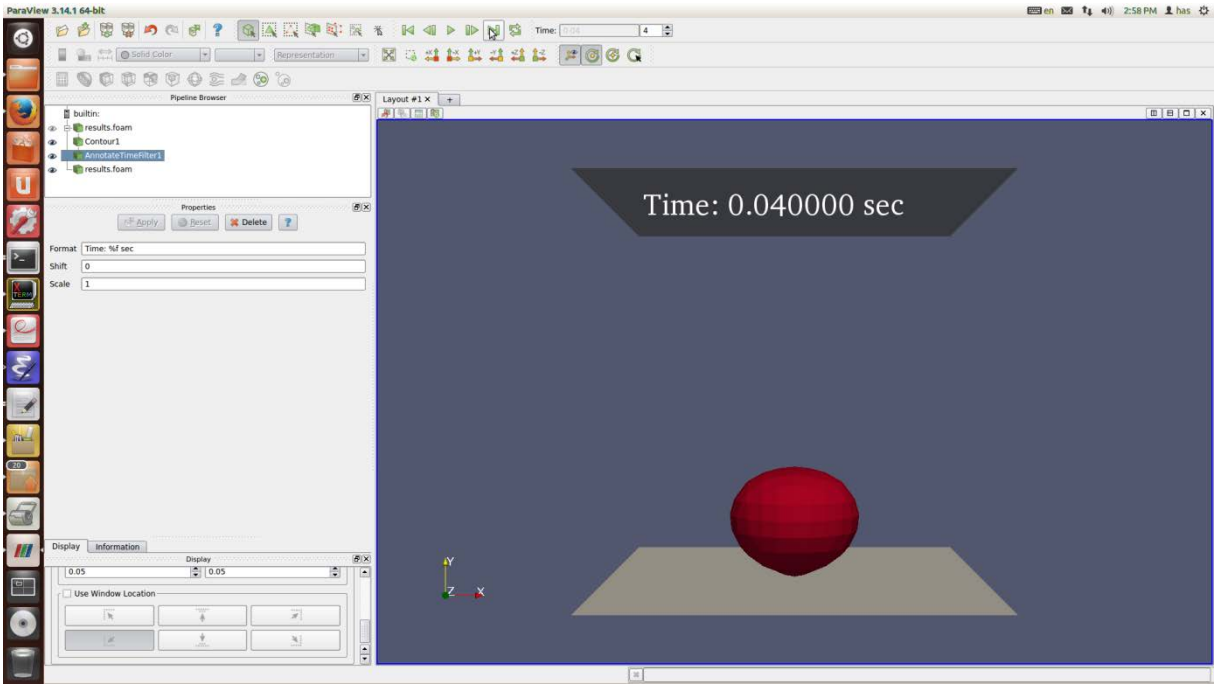


Figure 32: Post processing and visualization of the Nano printing process using SimPhoNy-paraview.

IX. Microfluidic application: Design tool for bubble-free nano- and micro-fluidic applications.

A proto-type application is developed for a multiscale design tool for bubble-free nano and microfluidic systems. The SimPhoNy environment is used as a development framework on top of which the application is developed. An advanced user interface component is developed to allow engineers to directly control relevant parameters, such as geometry, size distribution of the constituent's particles (cells, nano-particles, etc.). A specific component, SimPhoNy-UI has been developed to provide integration between different components together with a graphical user interface including pre and post processing based on MayaVI. While both bubble and particle (colloid) applications have been developed, the application user interface focused initially on the flow of particles in a bubble-free fluidic channel with an obstacle in the middle. This problem proved to be of general interest to the industry partners. The main goal of this deliverable is to provide an initial prototype system that shows the potential of exploitation of SimPhoNy in industrial applications.

The specifications of the application are derived and are determined during the project. The application couples discrete particle dynamics with continuum CFD models using an iterative coupling scheme, in which both models are solved for the same time step (concurrent multiscale modelling). SimPhoNy-UI integrates a LIGGGHTS and OpenFOAM wrappers hence the modelling of particles and fluid is performed with LIGGGHTS and OpenFOAM as backend engines (as solvers), while the coupling itself is performed within SimPhoNy framework itself. The bubble dynamics are modelled using the multiphase CFD model.

Due to the integration of Graphical User Interfaces and execution on remote servers, the simphony-UI is integrated with SimPhoNy-Remote providing a client server setup where bye the user configures and executes the simulation from within a web browser. A customized user interface is developed on top of MayaVi and Python allows the user to configure the parameters and setup of both particles and fluid components, as well as the coupling parameters. The user then can submit the job and monitor its progress from any browser connected with the server.

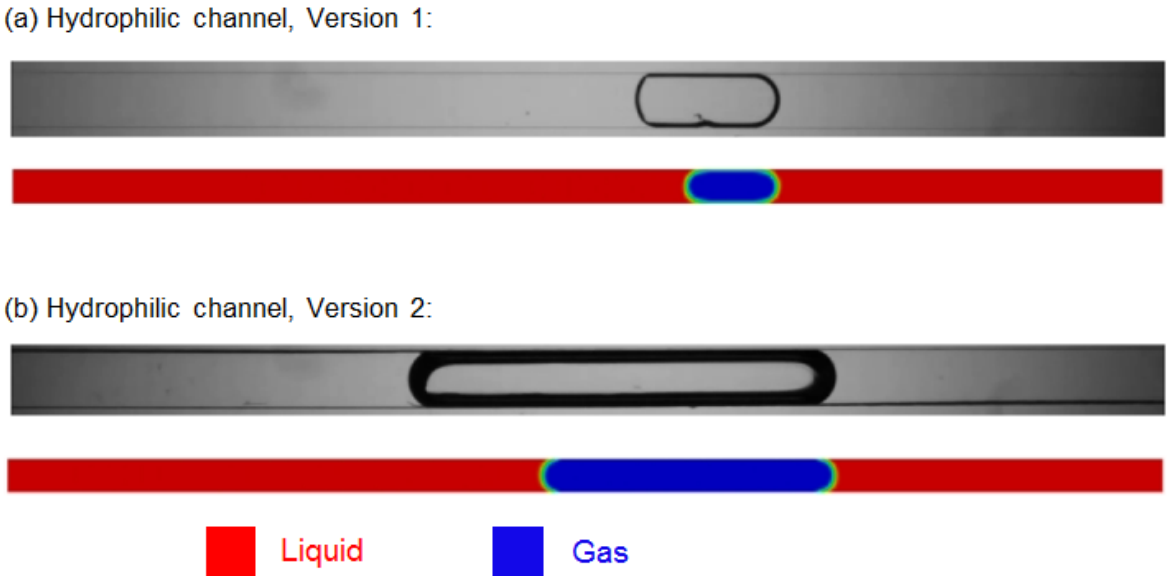


Figure 33: Validation tests for a single gas bubble flowing in a channel. Top image in each case is from experiments conducted by partner HEL and the bottom images are snapshots of simulations with SimPhoNy using the OpenFOAM backend engine. Special considerations of the dynamic and static wetting angle boundary conditions are needed to obtain realistic bubble shapes and flow.

Figure 34: A snapshot from the simulation application showing bubbles (grey colour) and liquid (dark). In the top figure it is shown how gas bubbles accumulate on the superhydrophobic surface (initially all bubbles are small like on the left of the figure). In the bottom figure it is shown how adding valves remove the accumulated bubbles to the outside.

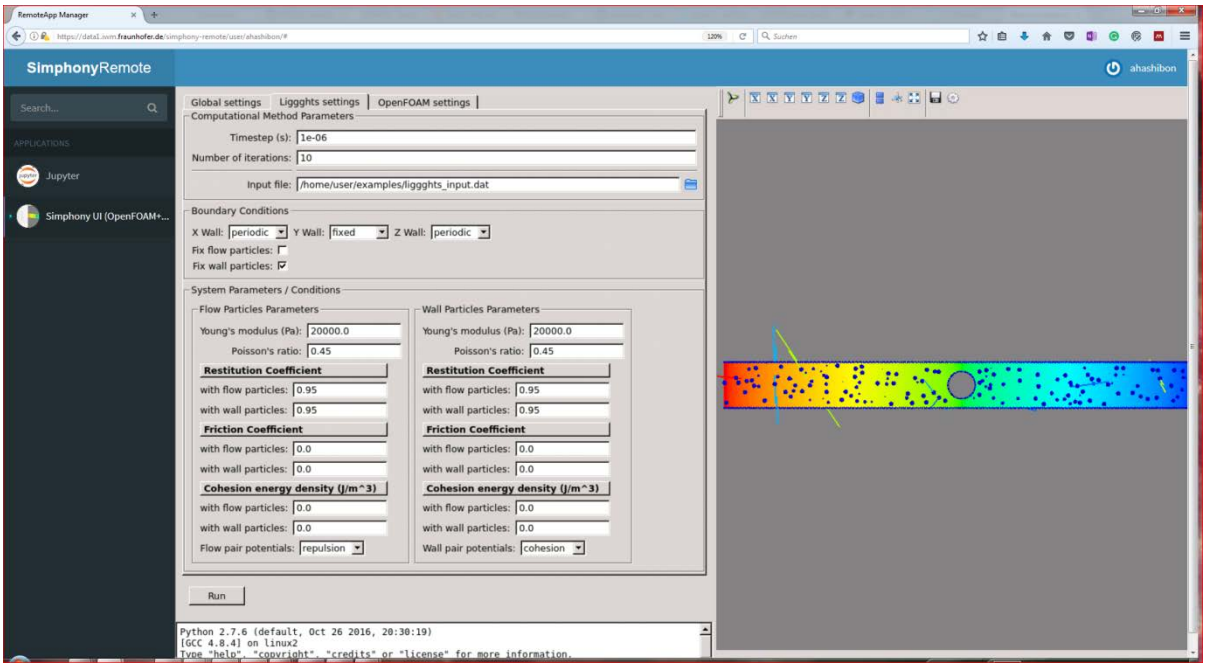


Figure 35: The SimPhoNy-UI interface inside an instance of SimPhoNy-Remote. Three tabs are offered to the user for setting up the CFD (OpenFOAM) and PD (LIGGGHTS) parameters as well as one for the coupling (Global settings). Note that while the UI shows explicitly the name of the integrated tools (LIGGGHTS and OpenFOAM) the actual coupling is performed using the SimPhoNy wrappers and CUDS.

X. Application for the design of foam-forming processes

The application focuses in particular on the rheological properties of aqueous foams and their influence on foam flows in pipe systems. The application involves a GUI for configuring, executing, and analysing simulations using the SimPhoNy framework. The GUI is provided by the *simphony-ui* module. The application runs in a dedicated server where a full installation of the SimPhoNy framework is maintained: the user obtains an access and controls the application via the *simphony-remote* module. A schematic description of the architectural system design is provided in Figure 36.

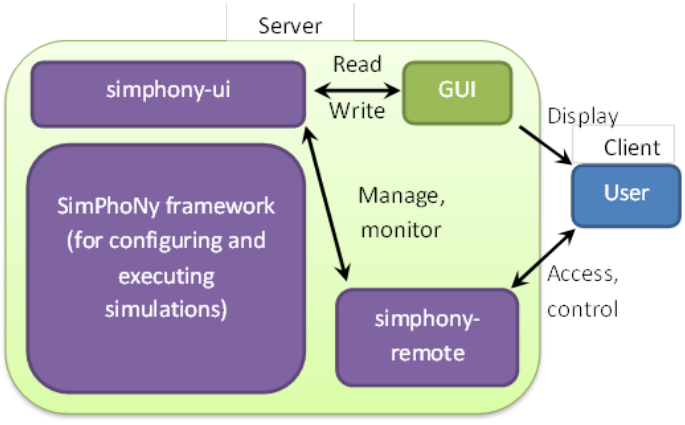
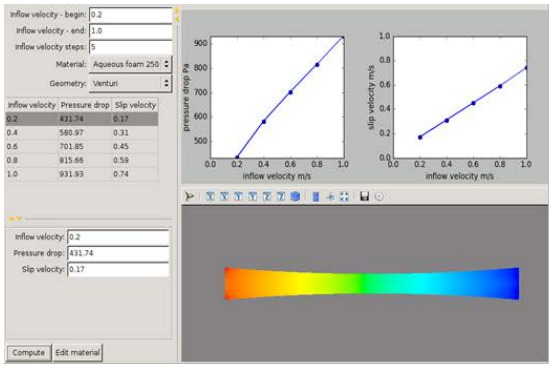


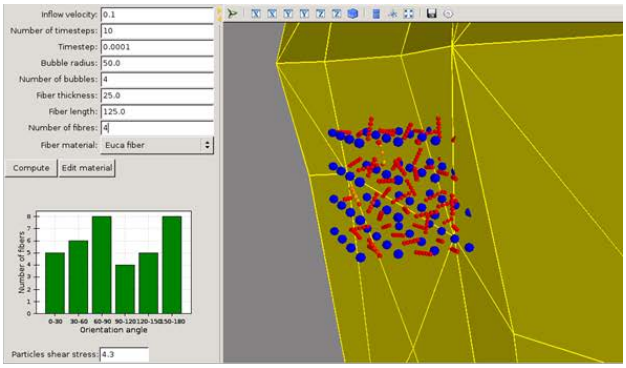
Figure 36: A schematic description of the architectural system design for the application

The application is decomposed into two parts designated as the *design engineer* and *material scientist* cases. In the design engineering case user can simulate fluid flows in various geometries relevant to foam-forming processes. Here the fluid properties and behaviour is modelled using the rheological Herschley-Bulkley model

together with a shear stress dependant boundary slip velocity model. By configuring the model parameters user can analyse, as a function of inflow velocity, the pressure drop between inflow and outflow boundaries as well as the average wall slip velocity (essential variables from a system engineering perspective). In the material scientist case fluid flows in a simple geometry are simulated. However, now the fluid properties are not determined using a rheological material model, but the properties are instead locally resolved from separate simulations on a much smaller scale (mesoscopic simulations). Specifically, at the small scale fluid-bubble-fibre suspension are simulated: the user can specify bubble and fibre properties which will then affect the bulk behaviour of the fluid and, ultimately, the emerging flow field.



Design engineer application



Material scientist application

Figure 37: Two parts of the foam-forming processes interface

Highlights of most significant results

- Experimental benchmarks have been conducted.
- Non-trivial sticking behaviour of droplets have been found on substrates.
- Three applications have been developed including user interfaces with substantial industrial impact.
- Educational application for NEMS have been setup.

The potential impact

SimPhoNy has eventuated in a large body of IP and achievements both in data science, software engineering and coupling and linking science. Despite the intensive dissemination activities, there is still unutilised potential for further publications and dissemination activities that will lead to further impact. A plan for dissemination, especially in open journals and conferences, beyond the project end has been put forward. These pertain mainly to the development of ontologies and related metadata as well as the applications and novel coupling and linking developed in SimPhoNy within the later period of the project.

Significant efforts in the present second (final) period are devoted to finalising the implementation of SimPhoNy, providing semantic knowledge management of materials modelling through the development of materials modelling ontology (contributing thus to the establishment of a European Materials Modelling Ontology (EMMO) and a standard for materials modelling and vocabulary), the development of an integrated framework that allows rapid development of novel advanced materials modelling workflows targeting key industrial applications is the main final result.

The developed CUDS data standards based on ontologies and common vocabularies impacts the steep learning curve associated with adaptation of novel advanced materials modelling in industry, especially in SMEs, as it makes it more straightforward to understand and quickly get acquainted with new modelling domains since the same vocabulary is used overall. It also impacts positively and contributes to the emerging domain of *material informatics* in the EU as it readily provides data and information that can be curated in databases and repositories and hence also contribute to open data and open knowledge in the EU and help integrate materials modelling into the digital single market (DSM).

Targeting the development of easy to deploy, maintain and operate modelling applications based on the SimPhoNy integrated Semantic framework allows advanced materials modelling workflows for the design of new materials and processes. It brings materials modelling closer to SMEs by reducing efforts to both maintain and learn new methods (and terms) and at the same time provides research institutes, modellers in general and software owners in particular new avenues to develop new custom tailored tools addressing the design of advanced products with tangible impact on European industries.

The SimPhoNy integrated framework enables rapid development and testing of new multiscale coupling and linking workflows, and as such it is expected to impact the whole field of materials modelling. In essence, SimPhoNy enables a democratisation of the development of concurrent multiscale and Multiphysics materials modelling taking it outside the exclusive realm of specialized labs and academics as it allows anyone to develop such paradigms. The demonstrated applications and apps are expected to be used in production environments by SME's to design new nano-printing, nano and microfluidic as well as novel foam forming processes. Extensions to other fields are straightforward.

Additional Impact Avenues

As additional impact avenues, SimPhoNy can contribute to increased utilisation of HPC infrastructure in the EU by the entire materials modelling community. Traditionally, HPC systems are targeted towards specifically developed codes utilising high performance algorithms that enable utilisation of the underlying HPC architecture to a maximum. As such, typical materials modelling software codes often need special extra tailoring and even rewrite of the bulk or entire algorithms for HPC resources. However, recent actions, especially within HPC at the European level (PRACE) are canvassing projects for new general applications that do not necessarily require customisation of codes to supercomputers. In this aspect, SimPhoNy consortium led by the CO will contact PRACE (e.g., Stephane Requena Chief Technical Officer at GENCI; Member, Board of Directors at PRACE) for showcasing SimPhoNy and its results on such platforms.

SimPhoNy educated staff can also act as additional avenues for future impact. Those former graduate (Master and PhD) students that find themselves in industry will surely consider the use of SimPhoNy and further interacting with the Consortium to build customized solutions. Furthermore, they may use the experience gathered, the knowledge of interoperability technologies and integration schemes to implement their own solutions, and thus SimPhoNy can even indirectly impact industry.

The following is a list of educated staff from SimPhoNy so far:

1. Tobias Rasp (Fraunhofer), PhD in materials science, worked on the CFD-DEM and CFD-MD coupling and is now employed by TRW Automotive (developers and producers of car safety equipment, such as Airbags and safety belts).
2. Nathan Franklin (Fraunhofer), MSc, worked on wrapper development and visualisation, is employed as a software developer at a research department at University of Texas at Austin.
3. Thomas Breinlinger (Fraunhofer), PhD, worked on the particle-fluid coupling, is employed by Bosch, doing various modelling of systems.
4. Mehdi Sadeghi (Fraunhofer), MSc, worked on wrapper development, now in industry (start-up).
5. Omar Salomón (CIMNE), Phd, worked on integrating Kratos, now is at CIMNE Technology (CIMNE subsidiary). Note: CIMNE cooperates with industry, hence the potential impact consists of bringing SimPhoNy based technology into additional markets.
6. Vantte Kilappa (JYU), PhD, worked on Lattice Boltzmann wrappers and common design, now at Aidon Oy, Finland (industry).
7. Veli Tuomas Turpeinen (JYU), Ph.D. worked on Lattice Boltzmann wrappers and common design, now at VTT Technical Research Centre of Finland Ltd (research support organization).
8. Ludwig Gutzweiler (BFX), PhD. Now at Hahn-Schickard Institute in Freiburg Germany (technology transfer).
9. Kit Yan Choi (ENT), hired by ENT to work on the project and remained at ENTHOUGHT as software engineer.
10. Seoung-Eun Kim (HELLMA), Dr.-Ing., worked on nano and microfluidic experiments as well as modelling, now at Neoperl GmbH.
11. Jeremy Rutman (IIT), Ph.D., worked on electronic models and wrappers, now in a startup in Tel Aviv.