IntOP 2015

The 3rd Workshop of the European Multi-scale Modelling Cluster: Interoperability in Multiscale Modelling of Nano-enabled Materials

Jyväskylä, Finland
28th–29th May 2015

Book of Abstracts

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Workshop venue

Lecture rooms FYS1 and FYS3 at the Department of Physics,
University of Jyväskylä, Ylistö Campus, Jyväskylä, Finland
Street address: Survontie 9, Jyväskylä

Scientific committee

Editors

Book of Abstracts edited by Vantte Kilappa and Keijo Mattila,
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May 21, 2015

Contents

Introduction

In modern physics, the evolution of computational capacity has allowed materials to be investigated in a wide range of length and time scales, generally referred to as multi-scale materials modelling (MMM). This allows for the modelling of complex materials under realistic constraints in a wide range of situation. Linking statistical methods to physical chemistry and electronic structure theory is necessary for simulating realistic processes in micro- or nano-scale components, and more importantly, allows for predicting material properties in addition to merely describing them.

Integrated Computational Material Engineering (ICME), on the other hand represents an industrial application of MMM. The discipline focuses on understanding how processes form material structures, how these structures give rise to material properties and how to select proper materials for applications based on this information. In essence, products are designed alongside the materials that comprise them, and the end result is investigated and simulated at multiple length scales during the product development.

The main challenge, both in MMM and ICME, is coupling and linking of models describing phenomena at different scales, from the nano-scale up to the device or macroscopic scale. Such challenge can be met by integrated frameworks that facilitate application of various multi-physics models in tandem and enable the predictive design of novel materials optimised for specified applications. Both disciplines are increasingly being recognized as vital components for a successful design of many novel nano-enabled products and enhanced production technologies, whose development could lead to great economic benefits.

Current computational tools typically have their own non-standard schemas for input and output files, including the definition of the model. At the same time, different communities often rely on distinct nomenclature to describe the same model components or physical parameters, which makes it even harder to link and couple disparate tools. Some existing tools use own metadata schemas, though these schemas are themselves distinct and translating from one to the other is not straightforward, time consuming and inefficient.

The IntOP2015 workshop is organized by 6 different EU supported projects and actions (SimPhoNy, Deepen, MoDeNa, NanoSim, MMP, ICMEg) which have the overarching goal to collaborate on developing data standards and interoperability interfaces for various tools and creating integrated multi-scale modelling environments for nano-enabled materials.

Here the interoperability relates to the ability to share data between different computer systems and programs. Interoperability can be achieved by creating a standard nomenclature and metadata based on taxonomy of existing models and tools. The basis is to establish a list of vocabulary that is universal in the sense that it can be used by all subdomains, and that is unified, in the sense that it brings all subdomains to use one common nomenclature.

The IntOP2015 workshop will cover recent developments in coupling and linking of models and methods for advanced nano-enabled MMM and ICME approaches in industry. A key goal of the workshop is to collaborate towards a common nomenclature and metadata proposal.

Schedule

Day 1, Thursday 28 May

8:45	**9:15**	**Workshop registration**
9:15	**9:30**	**Welcome & announcements**
Session 1		**Applications of Multiscale and Multiphysics Modelling in Material Science (chair H. Preisig)**
9:30	**10:00**	**P. Asinari (Invited talk): Standardization of Multiscale Materials Modelling Vocabulary** (30 min)
10:00	**10:20**	G. Schmitz (ICMEg): Microstructure modelling in ICME settings (20 min)
10:20	**10:40**	J. Hyväluoma (SimPhoNy): Multiscale simulations with LBM: dimensional analysis and time-scales (20 min)
10:40	**11:00**	P. Khomyakov (DEEPEN): Strained InGaAs ternary alloys and large-scale atomistic calculations (20 min)
11:00	**11:30**	Coffee break
Session 2		**Organising and Storing Data (chair T. Hagelien)**
11:30	**12:10**	**A. Gulans (Invited talk): NoMaD Repository** (40 min)
12:10	**12:30**	E. O'Reilly (DEEPEN): Databases and validation for modeling of III-N Electronic and Photonic Devices (20 min)
12:30	**12:50**	J. Adler (SimPhoNy): Visualization of electronic density of nanotube with AViz (20 min)
12:50	**13:50**	Lunch
Session 3		**Data Structures for Interoperability (chair E. Coenen)**
13:50	**14:30**	G. Schmitz (ICMEg): The hierarchical data format HDF5 (40 min)
14:30	**15:00**	A. Hashibon (SimPhoNy): CUDS and Vocabulary in the SimPhoNy Integrated Framework (30 min)
15:00	**15:20**	F. Sacconi (DEEPEN): HDF5 File-based interoperability for multiscale and multiphysics modeling (20 min)
15:20	**15:40**	**Discussion** (20 min)
15:40	**16:00**	Coffee break
Session 4		**From Data Structures to Modelling Platforms (chair E. O'Reilly)**
16:00	**16:40**	T. Hagelien (NanoSim): Porto, metadata and MongoDB data storage in NanoSim (40 min)
16:40	**17:00**	H. Rusche (MoDeNa): The MoDeNa multi-scale simulation software framework (20 min)
17:00	**17:20**	E. Coenen (MMP): Multi-scale modelling and simulations: a distributed and open-source platform (20 min)
17:20	**18:00**	**Discussion on multiscale cluster proposals on metadata** (40 min)
19:30	**22:00**	Workshop dinner

Day 2, Friday 29 May

Session 5		**Integration Approaches and Techniques (chair A. Hashibon)**
9:00	**9:40**	**A. Cepellotti (Invited talk): AiiDA framework and integration** (40 min)
9:40	**10:00**	B. Patzák (MMP): On Design of MMP Multiscale Modelling Platform (20 min)
10:00	**10:40**	H. Preisig (MoDeNa): Structured Ontology for Controlled Physical Processes (40 min)
10:40	**11:10**	Coffee break
Session 6		**Working on Proposal (chair Georg Schmitz and Gerhard Goldbeck)**
11:10	**12:00**	Open Panel Discussion on Cluster and platform proposal (50 min)
12:00	**12:30**	**Closure of the workshop, next workshop**

Session 1: Applications of Multiscale and Multiphysics Modelling in Material Science (chair H. Preisig)

P. Asinari	**Invited talk**	Standardization of Multiscale Materials Modelling Vocabulary
G. Schmitz	**ICMEg**	Microstructure modelling in ICME settings
J. Hyväluoma	**SimPhoNy**	Multiscale simulations with LBM: dimensional analysis and time-scales
P. Khomyakov	**DEEPEN**	Strained InGaAs ternary alloys and large-scale atomistic calculations

Standardization of Multiscale Materials Modelling Vocabulary

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Materials modelling is a strong activity in Europe and Europe plays a recognised leading role in the world. Yet, there is no organised European modelling community that represents all stakeholders. The European Materials Modelling Council (EMMC) is a community driven by bottom-up actions to connect all existing material modelling activities in Europe [1]. The EMMC aims at wide stakeholder consultation; to stimulate complementary activities to what already exists; to stimulate exploitation of existing materials modelling expertise; to stimulate model development necessary for industrial applications and to provide inputs for EC future visions/plans. The EMMC is proposing underpinning and enabling actions that will increase the industrial exploitation of materials modelling in Europe by identifying topics of Europe-wide interest: For example, see the EMMC Roadmap for Materials Modelling [2]. The activities proposed are to be developed from TRL3 to TRL7 to fit with the scope of the LEIT programme.

Clearly, connecting all existing material modelling activities in Europe requires a tremendous effort for systematically screening on-going projects. A Review of Materials Modelling has been written and describes modelling of materials, their properties and use in industrial applications illustrated by 100 FP7 Industrial Technologies NMP Materials and Nanotechnology projects [3]. This review revealed the urgent need for developing a common vocabulary across different modelling communities.

In this talk, I will present the current state-of-art in the above effort by highlighting the rationale behind the adopted classifications of this common language. For example, models are strictly classified according to the entity whose behaviour is described by the physics equation in the model and not according to the size of the application or system. In this way models are classified in four categories: electronic, atomistic, mesoscopic and continuum. These concepts are proposed to be used as highest level metadata and are essential prerequisites for the interoperability of models (multi-scaling) and databases.

References

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[3] Review of Materials Modelling, http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html, 2015.

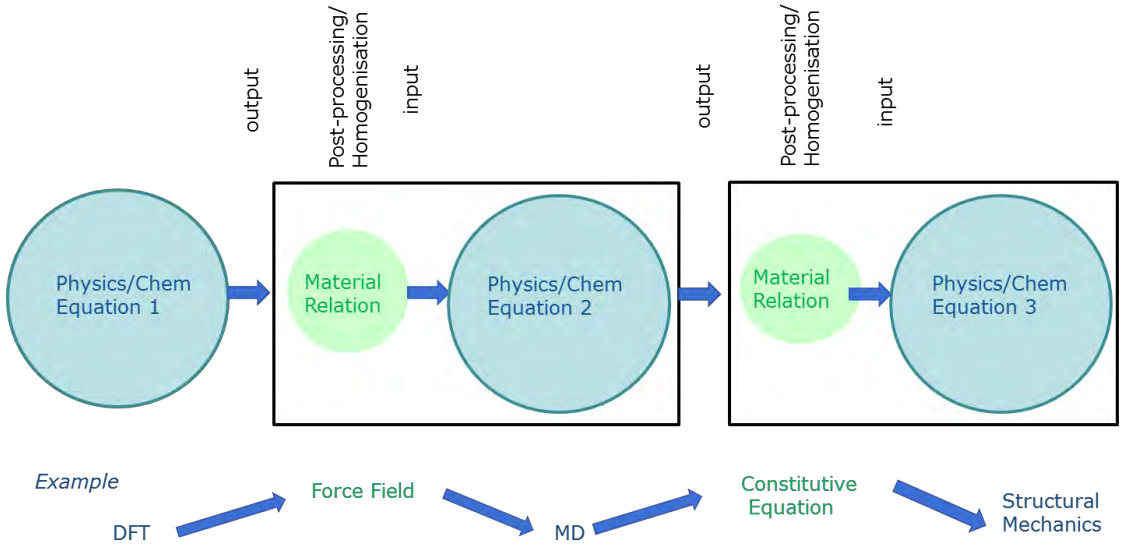

Figure. 1: Schematic view of a modelling hierarchy.

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Session 1

Microstructure modelling in ICME settings

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Microstructures and respective models for their evolution are at the borderline between continuum scale process models and electronic/ atomistic/mesoscopic models and thus provide a natural bridge between these different length scales. The role and needs of microstructure modelling in an ICME environment will thus be discussed with respect to their added value provided to macroscopic process simulations and their contribution to the prediction of materials properties.in more detail for the example of the multi-component, multi-phase field model MICRESS® [1].

Practical implications for coupling a heterogeneous variety of codes and tools to microstructure simulations will be discussed and the presentation will conclude with some conceptual thoughts about a future standard format for the description of digital microstructures, which should at least obey following conditions:

- free and powerful software tools should be available to inspect the digital microstructures
- the numerical representation should be easy and intuitive in view of educational aspects
- in spite of being easy and intuitive it must be sufficiently flexible and versatile for more complex tasks
- should make use of existing de-facto standards
- 2D representation should be a limiting case of a generic 3D representation
- should reflect the multi-scale nature of microstructure data
- …much more…

One path towards interoperability is the specification of a common data format. HDF5 [2] and VTK [3](as a part of HDF5) both meeting all above requirements have a strong potential to evolve into such a standard. Synthetic microstructures being generated with Dream3D [4] could already – without major effort - be further processed with MICRESS®.

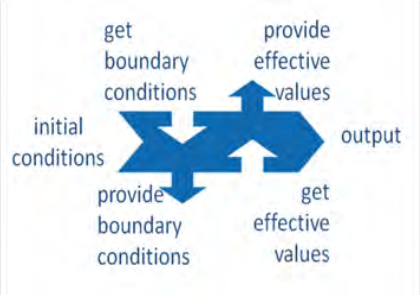

Figure. 1: Basic topology of a software tool in an ICME setting allowing assembling respective "puzzle parts" along the time/history and across the scales via exchange of boundary conditions and effective values [5].

Figure. 2: The "initial conditions" entering a microstructure simulation as initial microstructure may originate from a variety of sources. A similar variety of software tools serves the other arrows being depicted in fig. 1 [6]

References

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[2] http://www.hdfgroup.org/HDF5/
[3] http://www.vtk.org/
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[5] G.J.Schmitz and U.Prahl (eds) Wiley VCH, ISBN 978-3-527-33081-2 (2012)
[6] G.J.Schmitz et al. to appear Proceedings 3rd World Congress on ICME, Colorado, June 2015

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Lattice Boltzmann simulation of multiscale systems: Dimensional analysis and time-scale hierarchy

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Numerical simulation of multiphase fluid flows is a highly nontrivial task due to the spectrum of length and time scales involved: numerical stability and computational resources impose critical restrictions on the simulation parameters. For example, evolving interfaces are inherent in multiphase fluids. Interfaces form, move, and breakdown in response to viscous, surface, gravity, and inertial forces. The physical interface thickness is of the order of nanometers, i.e. a microscopic quantity, while the multiphase fluid features under investigation, like a droplet, are typically measured in micro- or millimeters. Hence, the *diffusive-interface model* is appropriate for studying very small scale phenomena and the *sharp-interface model* is a good approximation when considering dynamics at more macroscopic scales [1].

However, it can be computationally inconvenient, or even practically impossible, to utilize the sharp-interface model for multiphase flows, e.g., in confined or geometrically complex domains and when the interfaces experience large deformations or topological changes. An alternative is then to utilize the diffusive-interface model also at macroscopic scales by considering the interface thickness, now a macroscopic quantity, as a numerical artifact. The main challenge in this setting is to enforce correct values for the relevant material parameters, like surface tension, with the limited freedom in simulation parameters [2]. That is, the numerical simulation parameters are further restricted.

Similar challenges are encountered in simulations of particle suspension flows. Especially if the suspended particles are of colloidal size (particle diameter smaller than 1 μm), interactions induced by the surface charges of suspended particles and Brownian motion become important alongside the hydrodynamical interactions which dominate behaviour of suspensions of larger particle size. Thus various physical mechanisms taking place at many length and time scales are affecting the behaviour of colloidal suspension: the relevant time scales include hydrodynamical and Brownian ones as well as those related to the short-range interactions between electrically-charged colloids.

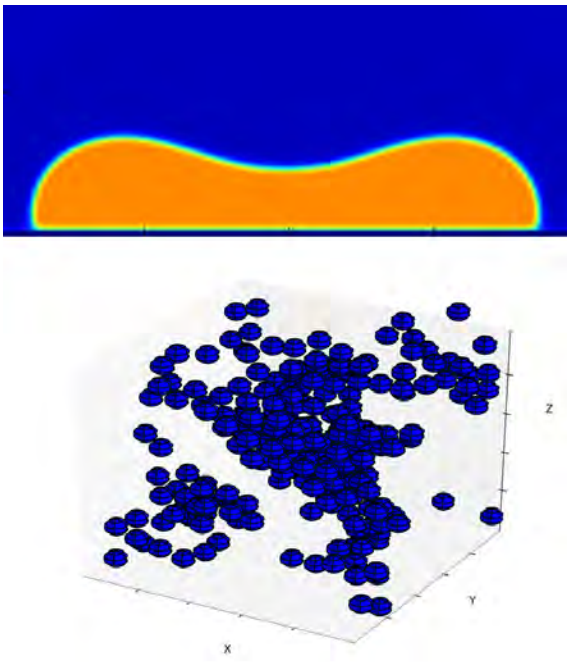

Figure 1: Applications used as examples: Droplet impact on a solid surface and shear flow of colloidal suspensions.

The relative magnitudes of the forces affecting the fluids and particles characterise multiphase flows. In fluid mechanics, dimensional analysis is frequently used to reduce the number of variables which affect a physical system, and to establish the relative importance of the involved physical mechanism. Dimensionless numbers can be presented as ratios of the appropriate characteristic time scales, and this allows one to estimate the range of those time scales that are most essential for the physical system and phenomena under consideration.

In practice, e.g. due to the above discussed reasons, it might be necessary to relax the hierarchy of time scales,

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which inevitably means that all dimensionless numbers cannot be matched between the simulation and the physical system. In other words, it is very difficult to reach a full dynamical similarity in numerical simulation of multiscale systems. Dimensionless numbers far from unity are especially problematic since the time-scale range to be covered by a simulation is wide.

Therefore, understanding on both the physical problem and the numerical method adopted is necessary to achieve reliable simulation results. Understanding on the physical problem is needed when simulation parameters and dimensionless numbers are tuned to maximize the simulation efficiency. In such tuning some of the time scales inevitably become unrealistic whereby it is essential to be aware which processes are not described correctly on a quantitative level. Understanding on the numerical method is, on the other hand, important in order to ensure that simulations are not carried out with invalid numerical parameters.

Here we exemplify the above matter by means of the lattice Boltzmann method and two specific applications which are impact of microdroplet on a solid surface and shear flow of colloidal suspensions. In droplet simulations Shan–Chen multiphase model with Peng–Robinson equation of state is utilized [3, 4]. Suspended colloids are modelled as point-like particles and their interactions are described by the DLVO theory [5]. In both cases we consider the essential physical processes, respective time scales, and their relations to the dimensionless numbers used to characterize these flows.

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Compositional dependence of the electronic, structural and mechanical properties in strained InGaAs ternary alloys: large-scale atomistic calculations

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III-V semiconductor compounds are considered for the integration with Si-based microelectronics to take advantage of their high charge carrier mobility [1]. This drives basic and applied research on various aspects of the III-V semiconductor materials as well as on the device design [1,2]. One field of extensive research is to understand how the electronic properties of the III-V compounds are altered by stress that is externally applied to tailor characteristics of semiconductor nanodevices [1,3]. Though the III-V compounds are material systems of high relevance, many of their properties have not been well understood because of a high complexity of the random alloy structures. A reliable prediction of alloy properties requires a multiscale approach to describe the alloy disorder effect on physical parameters.

Using large-scale atomistic, density functional theory calculations, we study in a systematic manner how the physical properties of the strained InGaAs ternary alloys depend on the scale of atomistic modeling. The electronic structure of these ternary alloys has been calculated within the framework of local density approximation and hybrid functional approach for relatively-large cubic supercells and moderate-size special quasi-random structures, which represent two kinds of model structures for random alloys. In particular, we show that conduction and valence band energies and their deformation potentials exhibit a non-negligible effect of compositional bowing in strained ternary semiconductor alloys such as InGaAs. The predicted bowing effect is found to be rather insensitive to the choice of the functional and alloy structural model. The direction of bowing is determined by In cation atoms that give a stronger contribution to the formation of the InGaAs valence band states, compared to Ga cation atoms. We also find that the heavy hole mass as well as the electron mass at the X and L valley minima severely suffer from the finite-size effect.

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Session 2: Organising and Storing Data (chair T. Hagelien)

A. Gulans	**Invited talk**	NoMaD Repository
E. O'Reilly	**DEEPEN**	Databases and validation for modeling of III-N Electronic and Photonic Devices
J. Adler	**SimPhoNy**	Visualization of electronic density of nanotube with AViz
J. Adler	**SimPhoNy**	AViz - Atomistic Visualization

Note: There are two abstracts by J. Adler, but the related topics will be covered in a single presentation.

On the search for novel materials: From evaluation of methodology to insight by sharing

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On the steady search for advanced materials with tailored properties and novel functions, high-throughput screening is a new branch of materials research. For successfully exploring the chemical compound space from a computational point of view, two aspects are crucial. These are (i) reliable methodologies to accurately describe all relevant properties for all materials on the same footing, and (ii) new concepts for getting insight into the materials data that are produced since many years with an exponential growth rate.

Concerning (i), I survey our benchmarking efforts in electronic-structure theory. With vast amounts of data produced employing different codes on different approximation levels, it is important to have a reference method. It requires that the Kohn-Sham equations are solved without any approximation besides those inherent to the chosen density-functional-theory functional. We have developed a framework for such reference calculations employing the `exciting14` code [1] that implements the full-potential linearized augmented plane wave method. Using this approach, an impressive precision of 1 $\mu\mathrm{Ha/atom}$ is reached for absolute total energies in a representative set of atoms and solids. After having demonstrated the credibility of the exciting code as a reliable benchmark tool, I present our results [2] for the test set consisting of 71 elements of the periodic table [3].

The NoMaD Repository [4], promoting the idea of open access and sharing of materials data, serves purpose (ii). As open access implies that data can be used by anyone, large collections of materials data opens an avenue for using and developing tools that the present computational-materials community does not even know.

To make the link between these two areas, I outline one of the next steps [5] of the NoMaD Project. How to make data comparable, i.e., independent of the underlying electronic-structure code? I argue that by achieving this goal, the significant information content inherently inside all materials data can be optimally exploited.

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[5] http://NoMaD-Lab.eu.

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Session 2

Session 2

Database development and validation for modeling of III-N Electronic and Photonic Devices

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The importance of nitride-based materials was recognized with the award of the 2014 Nobel Prize "for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources". Surprisingly, there are still many aspects of these materials which are not well understood. Despite the progress to date, there remain many challenges: not just to further enhance the efficiency of blue LEDs but also to develop LEDs that emit efficiently across a wider spectral range, as well as to develop III-N heterostructures for high power electronic applications. Further progress requires not just materials development but also the input of theoretical modelling to analyse and guide the development of optimised devices.

We are addressing the several scales of model required to describe key details of the electronic structure of III-N materials, and its consequences for device design and analysis. Many of the electronic properties of III-N structures are dominated by the large built-in polarization potentials found in such materials, and also by the impact of random alloy effects on the electronic states. *Ab-initio* techniques based on widely available density functional theory codes provide key III-N material parameters [1,2]. However, the accurate treatment of random alloy effects typically requires empirical atomistic models that include of the order of 10^5 atoms in the calculation [3,4]. This is illustrated in Figure 1, which shows the variations in local polarization potential in an InGaN/GaN quantum well structure, calculated using a set of "*bespoke*" atomistic models that we have developed. The full analysis of III-N devices requires treatment of even larger structures, typically carried out using continuum models, often based on using **k.p** or effective mass models, and implemented using commercial drift-diffusion and related methods [5]. The input data for such device-level calculations typically comes from a combination of *ab-initio* and empirical calculations, as well as from direct experimental measurements.

Based on our experience of developing models for III-N nanostructures, we discuss the requirements and likely development of genuinely open-source databases for material and device modelling. Of the three model types discussed above, steps are already underway for the development of open-source databases for parameters derived from *ab-initio* codes. There are already well established (primarily publication-based) routes for the presentation of input parameters for empirical atomistic and continuum-based electronic structure models. We argue however that because of the more "*bespoke*" and/or commercial nature of empirical models it is likely that fully open-source databases related to such models will lag behind those for *ab-initio* codes. We conclude by discussing briefly routes towards the development and achievement of such databases.

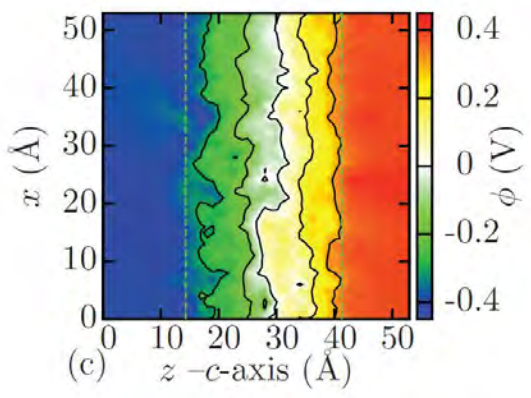

Figure. 1: Variation of local polarization potential in an $In_{0.3}Ga_{0.7}N$/GaN quantum well structure.

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Visualization of electronic density of nanotube with AViz

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The spatial volume occupied by an atom depends on its electronic density. Although this density can only be evaluated exactly for hydrogen-like atoms, there are many excellent algorithms and packages to calculate it numerically for other materials. Three-dimensional visualization of charge density is challenging, especially when several molecular/atomic levels are intertwined in space. In a recent project, we explored one approach to this: the extension of an analglyphic stereo visualization application based on the AViz package for hydrogen atoms and simple molecules to larger structures such as nanotubes. I will describe these techniques and demonstrate the use of analyglyphic stereo in AViz, [1, 2].

The use of AViz dot-mode visualization for electronic density was first developed in an undergraduate project about the hydrogen atom[3]. We then visualized the electronic density resulting from simulations of larger molecules and solids in the same way. Further studies [4] used a density functional theory approach to examine the electronic densities of simple molecules where there is no analytic solution.

The next stage in our visualization development was to move to 3D stereo. Stereo Vision (SV) works by showing a different image to each eye, thus creating the illusion of a 3D image. AViz 6.1 [1, 5] incorporated the possibility of SV, and although more than two colors are possible there remains some color washout, depending on color selection. The SV images generated by AViz, are best viewed using red-cyan anaglyphic glasses. An example of a simple stereo nanotube atomistic visualiztion is given in Figure 1. Stereo Visualization was applied to the electronic density of the hydrogen atom by Meital Kreif in [6].

The width of a nanotube wall is an essential parameter in order to scale up atomistic simulations into continuum models. In order to measure this, one needs to calculate the electronic density. For this calculation we selected the public domain code Quantum Espresso (QE) plane-wave DFT code [7] which has clear documentation of their format for the charge density. We chose the

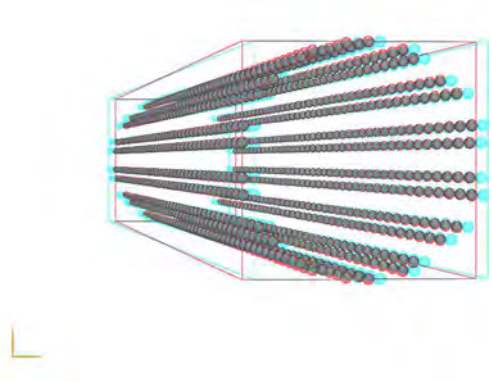

Figure 1: SV of nanotube.

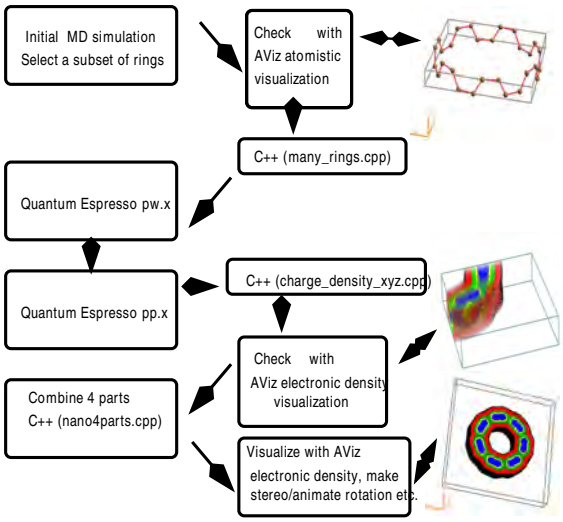

Figure 2: Flow chart of visualization procedure.

vdW-DF non-local correlation functional with the C09 [8] exchange functional in order to account for London dispersion interactions (or van der Waals forces) within

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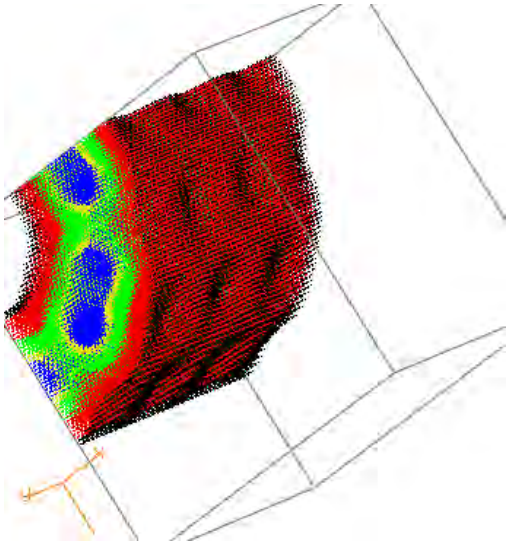

Figure 3: Enlarged view of 1/4 of the system.

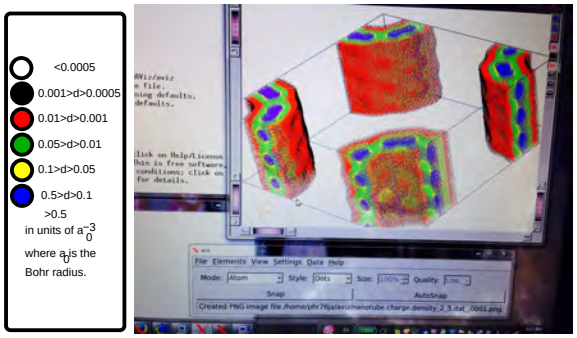

Figure 4: Color key to different electronic densities (left) and a screen shot of AViz in action (right).

our calculations.

The procedure for processing the QE output into AViz is described in [9], including all QE scripts and visualization technicalities. We found that color binning and some random dilution optimises the possibility of "transparency" into the samples. A flow-chart of all steps is shown in Figure 2, an enlarged image of 1/4 of the system is given in Figure 3 and the color code for different densities (d) in these two figures is given in Figure 4. This color palette was optimised for clear distinction between densities. A different palette optimised for stereo viewing is shown in Figure 5, with an animated version at [9].

Acknowledgements: This study is part of the EU-SimPhoNy project and provides one of the use cases. VRC was supported by the US DOE, Office of Science, BES-MSED.

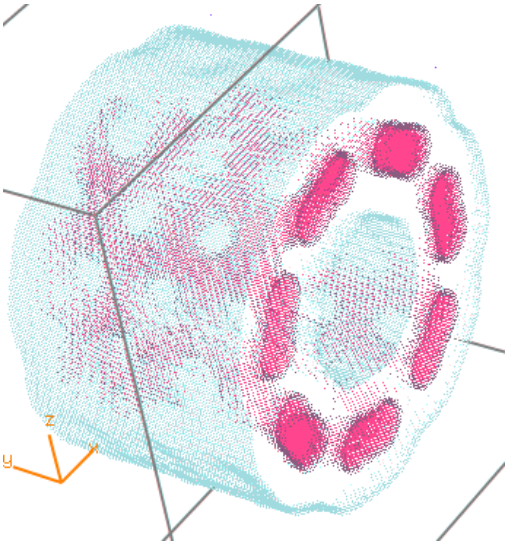

Figure 5: Stereo view.

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AViz - **A**tomistic **Viz**ualization

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Figure 1: AViz homepage

AViz, [1, 2] is a C++ and OpenGL/mesa based public domain package designed to visualize large numbers of atoms, vector spins, quadrupoles and other solid objects. Its application in dot mode to the visualization of electronic density is described in a companion abstract, here we concentrate on visualization of three dimensional systems of solid objects, whose locations and (where applicable) directions or polymer connections are calculated in advance or in parallel with a wide range of simulation or enumeration tools.

AViz differs from many other excellent existing visualization tools in that it was created by physicists interested in the study of defects, amorphous systems and sample melting with the philosophy that no predefined bond lengths, connections or angles exist. Bonds are actually concentrations of high electronic density, but the basic information concerns object locations (and directions if the object is a spin or a quadrupole). Cylindrical bonds can and are constructed as a guide to the eye for depth comprehension, or drawn to aid recognition of localpe. atomic coordination, but are only one of many tools for helping to understand sample structures.

The latest version of AViz can be found on the SimPhoNy github pages [2] and a new website [1] contains examples and tutorials. Within the framework of SimPhoNy effort has already gone into streamlining the source compilation process, and in material to support installers who may not be systems experts. Tutorials both on general AViz' use and on applications to nanomaterials such as nanotubes are being developed, [3]. Nano-related examples are shown in Figure 2, where the use of slice-indicate-only and of bonds of specific sizes are invoked to illustrate nanotube bending. In Figure 3 two applications of color variation are presented to identify defects [4] and illustrate layer mixing in melting magnesium, [5] In Figure 4 we give an example of color variation for different carbon hybridizations, [6].

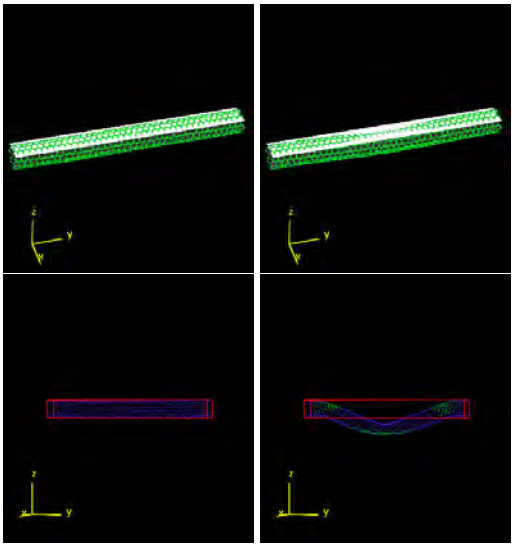

Figure 2: Techniques to highlight nanotube bending, slice-indicate-only (top) and coloring bonds of specific lengths only and retain viewpoint (bottom)

Sometimes, in order to show lattice structure, we may wish to only draw lattice bonds, and sometimes a sim-

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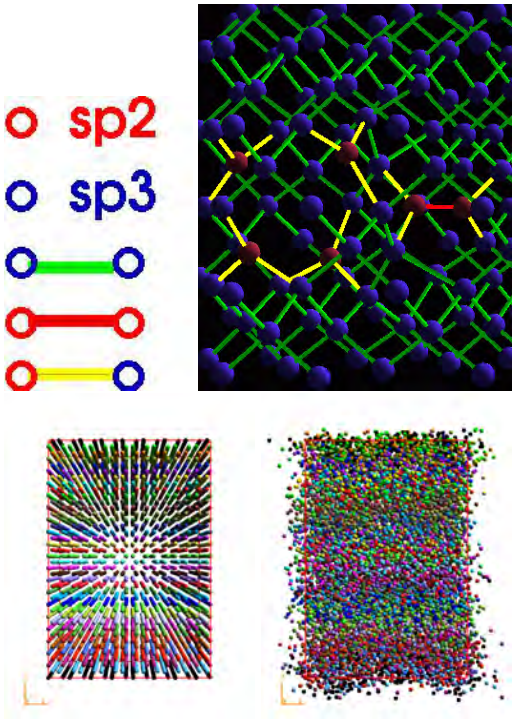

Figure 3: Use of color to show defects (top) and layer mixing (bottom)

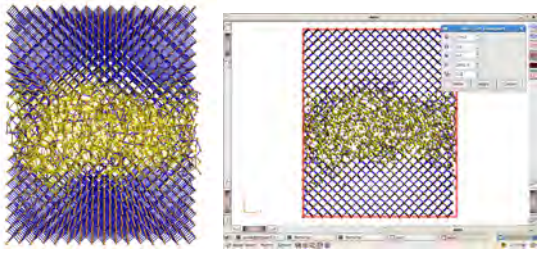

Figure 4: Graphitization to enable etching for diamond membranes, image at right with adjusted fovy

ulation model has non-atomic alternative objects such as spins [7] or liquid crystal [8]. We might want to retain the connectivity of a polymer (wrapped around a nanotube in this case). In Figure 5 we present images from such examples. In both the spin and liquid crystal cases color is used to indicate direction through an AViz panel, whereas in the other images color is preselected and introduced via the elements panel.

AViz has many options, and is especially useful for projects with interaction between computational experts and laboratory experimentalists, because it enables translation between different worldviews with the universal language of visualization. However, until now it is only available in LINUX, and its installation was a little complex. In the framework of SimPhoNy, efforts have been made to clean up the code and simplify the installation, with files on Github [2] and plans to provide versions for other systems are on track.

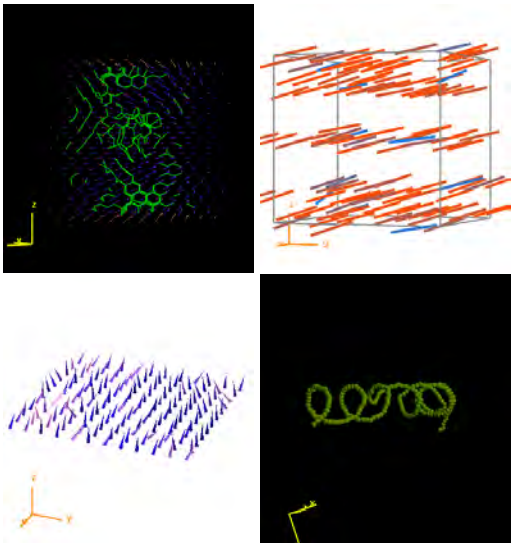

Figure 5: Different examples: Diamond transformed to graphite (upper left), liquid crystal (upper right, from [8]) spin visualization (lower left, from [7]), a polymer wrapped around a nanotube (lower right)

Acknowledgements: Further development of AViz is part of the EU-SimPhoNy project and relates to several of the use cases.

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Session 3: Data Structures for Interoperability (chair E. Coenen)

G. Schmitz	**ICMEg**	The hierarchical data format HDF5
A. Hashibon	**SimPhoNy**	CUDS and Vocabulary in the SimPhoNy Integrated Framework
F. Sacconi	**DEEPEN**	HDF5 File-based interoperability for multiscale and multiphysics modeling

The hierarchical data format (HDF5) - a basis for improved interoperability ?

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This presentation will discuss the "Hierarchical Data Format" (HDF5) as a basis for improved interoperability between the heterogeneous variety of simulation tools in the area of computational materials engineering at all length scales.

Following a short history of HDF5, some areas of applications of HDF5 in continuum engineering will be shown. In the following, the "customization of HDF5 to materials modelling" as realized in Dream3D will shortly be highlighted including some on-line demonstrations.

Eventually some relevant basics of the HDF5 data structure, fig. 1, will be explained and their potential to generate a structured list for attributes and fields as a basis for a metadata keyword list will be discussed.

Cell data represent the smallest bit of information and are especially used to describe properties „continuously" varying in space (called fields in mathematics).

Field Data – not to be confused with the mathematical fields above – describe properties which are identical for a given grain which is defined as a "field of voxels" belonging to the same object/grain and being specified by the same GrainID.

Ensemble data describe properties which are common to a number of objects like a number of grains all belonging to the same phase. A special type of ensemble data – not currently explicitly specified in Dream3D - would be *RVE data*. RVE data correspond to the ensemble data of all objects in the RVE and describe properties of the entire RVE.

This presentation is meant to kick start the discussion about and the work on a list of metadata keywords, which shall proceed interactively. For this purpose the audience is requested to bring along their PC with Excel being installed.

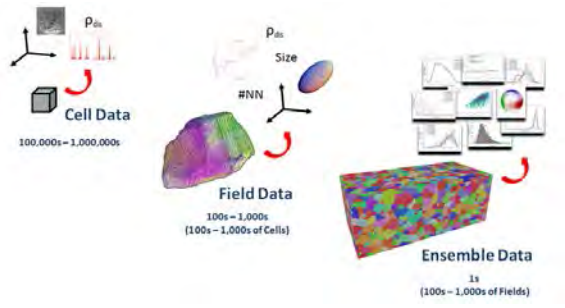

Figure. 1: Basic structure of HDF5 comprising "cell data", "field data" and "ensemble data". For explanations see text. The figure has been taken from the Dream3D manual [2]

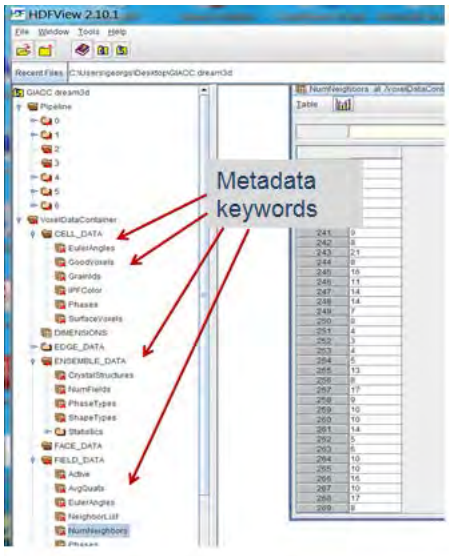

Figure. 2: Example of a HDF5 file being customized for the description of materials. Data are visulised with HDFview [1]

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Common Universal Data Structures (CUDS) and Vocabulary in the SimPhoNy Integrated Framework

Adham Hashibon[1†], Nathan Franklin[1], Tobias Rasp[1], Ioannis Tziakos[2], Didrik Pinte[2], Pooyan Dadvand[3,4], Carlos Roig[4], Keijo Mattila[5], Tuomas Puurtinen[5], Kai Hiltunen[6], Guillermo Román-Pérez[7], Gregorio Garcia[7], Joan Adler[8]

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Advanced nano-enabled materials exhibit complex behaviour at all scales. Designing new materials requires that all properties are considered, down from the electronic and atomistic scales, where the atomistic arrangement and chemistry are relevant, to the micro-meter scale, where effects of extended defects and the microstructure are of concern, up to the macroscopic, device scales. Traditional multiscale approaches relay on separating the system into subdomains, each modelled separately by a suitable single scale method. Linking (hierarchical and sequential) and coupling (concurrent) multiscale models are then needed to allow for the information passage between subdomains. However, while numerous modelling methods and tools exists for modelling a material at a single scale, e.g., LAMMPS, Quantum ESPRESSO, or OpenFOAM, there is currently no well-established multiscale tools and approaches that can, for example, be easily adopted in Integrated Computational Material Engineering (ICME) tool chains. This is mainly due to the difficulty of designing monolithic multiscale applications that allow describing the material accurately at each subdomain or scale and at the same time enable the necessary linking and coupling. An integrated multiscale framework that facilitates interoperability between single scale available tools is therefore of great importance for designing new materials and devices, especially for nano-enabled systems.

Interoperability relates to the ability to share data between different computer systems and programs. Different tools in use today have their own non-standard schemas for input and output files, including the definition of the model. Different communities use often distinct nomenclature to describe the same model components or physical parameters, which makes it even harder to link and couple disparate tools. Some existing tools use own metadata schemas, though these schemas are themselves distinct and translating from one to the other is not straightforward, time consuming and inefficient.

Interoperability can be achieved by creating a standard nomenclature and metadata based on taxonomy of existing models and tools. The basis is to establish a list of vocabulary that is universal in the sense that it can be used by all subdomains, and that is unified, in the sense that it brings all subdomains to use one common nomenclature.

In the SimPhoNy integrated framework, a list of Common Universal/Unified Basic Attributes (CUBA) has been created to facilitate the information passage and representation of models and data between all subdomains. CUBA is then augmented with Common Universal/Unified Data Structures (CUDS) that have a specific schema for data presentation. The CUBA can be considered as special CUDS keywords which are the basis of the metadata model. The CUBA and CUDS are represented both as a set of high level specifications and as a specific implementations using YAML syntax metadata and Python Wrappers, respectively.

On the low level, the CUBA specifies a basic knowledge-based set of keywords that cover all aspects of the models and associated numerical computational methods. For example, temperature is a fundamental concept that is used in numerous models in different contexts. In continuum models it is the macroscopic thermodynamic temperature of a whole domain or on specific mesh elements. While for atomistic systems it may be the local kinetic

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temperature or a global parameter defining the interaction with a thermal bath. It can be associated therefore with either a parameter of the system or a variable. In either case, one CUBA keyword is associated with temperature in SimPhoNy with appropriate basic metadata. This metadata is then augmented with the associations and relations between different model components to obtain readily the exact nature of the particular temperature and its context in the model. The SimPhoNy metadata is not constrained only to the variables of the state data (SD), but cover the system parameters and material relations (SP) (which is basically the *model*, i.e, the set of governing equations and material relations [1]), boundary conditions (BC) and computational methods (CM). An up-to-date list of the CUBA and CUDS can be found on GitHub [2]. All components of the SimPhoNy model are set and defined through CUBA and its related metadata and represented in CUDS.

The particular translation or information transfer from each integrated tool to SimPhoNy and back is accomplished through specific software interface wrappers developed for each tool. The wrappers communicate with the tools by either reading or writing the tool's native data files (FILE-IO) or by using the tool's library interface to have access to the internal state of the application. The wrappers return high-level container objects (which are part of CUDS) that act as a proxy for the users to update or query the internal representation stored inside the wrapper and modelling-engine. This enables, as shown schematically in Figure 1, the seamless transfer of data and models from one tool to another. A special feature of the SimPhoNy wrappers is that the data from all models share the same standard interface and one can move the data from one wrapper to another sequentially avoiding thus network saturation. In this way, SimPhoNy provides a direct seamless interoperability between all tools through the CUDS interface.

The SimPhoNy project has also created an HDF5-based file format to store the CUDS objects, relying on the CUBA keywords that include the whole model components: SD, SP, BC and CM. The SimPhoNy framework includes an H5CUDS class which implements high-level container objects using the standard interface of CUDS to provide the user a uniform way to access the objects stored in the files. For HDF5-file access, the H5CUDS class and associated classes use the PyTables [3] package which is based on HDF5 and provide for optimized handling of large tabulated datasets. As the H5CUDS file is an HDF5 file with an open description, it can also be accessed using any HDF5-supported APIs and other 3rd party tools.

In addition to interoperability and standard data formats, SimPhoNy provides a powerful development environment for multiscale science. It enables coupling and linking of Molecular Dynamics, Computational Fluid Dynamics, Lattice Boltzmann methods, as well as Density Functional Theory models. This is currently achieved through the integration of LAMMPS, OpenFOAM, Numerrin, JYU-LB, KratosCFD and KratosDEM, and Quantum ESPRESSO. Additionally several visualisation and pre/post processing tools, such as AViz, Mayavi, nCAD and nCAD-fluid, are also integrated in the same manner.

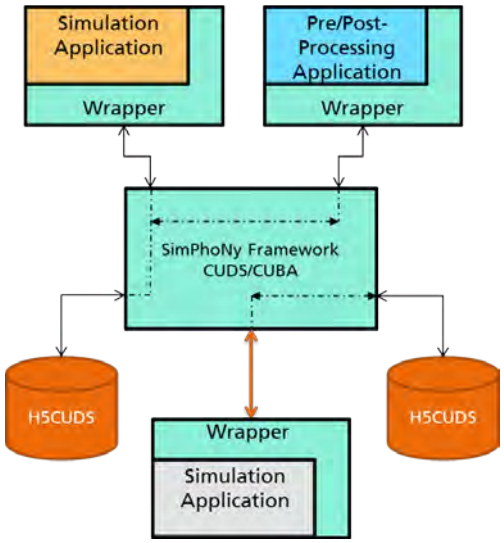

Figure 1: An example of the SimPhoNy design. The wrapper provides a common API to all integrated components and provides CUDS as a standard interface for data and models. Data can be moved from one component to another through the use of the SimPhoNy framework and CUDS. Data can also be stored in H5CUDS files.

Acknowledgements: The SimPhoNy Project received funding from the European Union Seventh Framework Programme (FP7). Grant number 604005.

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HDF File-based interoperability for multiscale and multiphysics modeling

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An Open Source software environment for the multiscale simulation of electronic and optoelectronic devices is being developed in the FP7 Project "From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures" (DEEPEN) [1].
The aim of the project is to develop an integrated multiscale simulation capability for predictive design of novel materials and nanostructures, such as LEDs based on InGaN/GaN nanowires and InGaN/(Al)GaN quantum wells, as well as nano-scale electronic devices including new channel materials for sub-10 nmCMOS. The software tools employed for multiscale simulations in this project will be integrated in the OS grid middleware environment UNICORE, by implementing suitable interfaces for the exchange of data and the coupling of simulations. An open source Common Data Format (CDF) has been defined to allow the exchange of data of different kind in the framework of the OS software environment. The CDF has been implemented based on the existing open source standard Hierarchical Data Format, HDF5 [2]. Together with the CDF, the related input/output (I/O) application program interfaces (API), which provides methods for reading and writing data used in the project, have been developed. The Hierarchical Data Format (HDF) has many important characteristics for scientific data storage. It offers platform-independent binary data storage with optional compression and hierarchical data ordering. Data are stored with alphanumeric tags, so that one can examine a HDF5 file's contents with no knowledge of how the file writing program was coded. The Hierarchical Data Format (HDF) implements a model for managing and storing data (see Fig.1). The model includes an abstract data model and an abstract storage model (the data format), as well as libraries to implement the abstract model and to map the storage model to different storage mechanisms. The HDF5 library provides a programming interface that allows a concrete implementation of the abstract models. Abstractly, an HDF5 file is a container for an organized collection of objects. The objects are groups, datasets, and other objects in a hierarchical structure. The objects are organized as a rooted, directed graph. Every HDF5 file has at least one object, the root group. All objects are members of the root group or descendants of the root group.

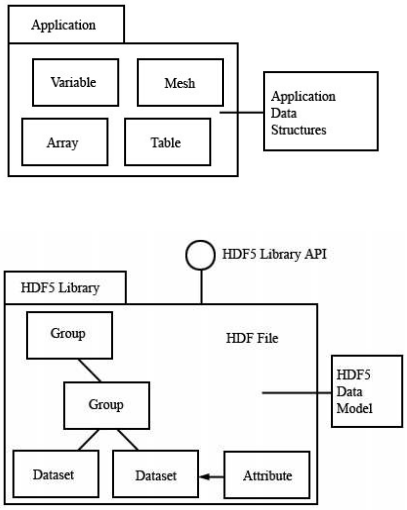

Figure. 1: HDF Data Structure at different layers.

For example a HDF group contains zero or more objects, and every object must be a member of at least one group. An HDF5 dataset is a multidimensional (rectangular) array of data elements. The shape of the array (number of dimensions, size of each dimension) is described by the dataspace object.
We can conclude that HDF file format provides several features which can make it a good choice as a common data format for interchange of material data through different simulation tools, such as:

- Platform-independent binary data storage with optional compression
- Hierarchical data ordering
- Self-describing tags
- Support for complex data relationships and dependencies through Datasets (multidimensional arrays) and Groups (container structures)
- Direct access to parts of the file without first parsing the entire contents
- Efficient support for a parameter database
- Possible embedding of post processing of output results, data plots, etc.

References

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[2] www.hdfgroup.org/HDF5

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Session 4: From Data Structures to Modelling Platforms (chair E. O'Reilly)

T. Hagelien	**NanoSim**	Porto, metadata and MongoDB data storage in NanoSim
H. Rusche	**MoDeNa**	The MoDeNa multi-scale simulation software framework
E. Coenen	**MMP**	Multi-scale modelling and simulations: a distributed and open-source platform

Porto: A framework for information interchange and multi-scale fluid mechanics simulations.

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Key words: Meta-data, Information Interchange, Software Framework, JSON, MongoDB

Abstract. We present our strategy and implementation of a data centric framework with focus on information interchange for multi-scale fluid mechanics simulations. We propose a schema for defining meta-data for possible standardization for the Multiscale Cluster/ICMEg consortium. Within the NanoSim consortium, WP1 deals with defining a framework (Porto) for connecting and utilizing software simulators of different scales through offline-coupling. The focus of engineering applications within the NanoSim project is fluidized beds. For such large-scale applications the most promising multi-scale simulation strategy is to focus on representative elements of the simulation domain, resolving these representative elements on a small scale, and feed the result into a sub-grid model on the next larger scale. Within NanoSim, the following 6 scales are accounted for:

- System scale, simulated by a system of Ordinary Differential Equations (ODEs)
- Equipment scale, simulated by Large-Scale Computational Fluid Dynamics (CFD) Simulations
- Cluster scale, simulated by coupled CFD-DEM (Discrete Element) simulations
- Particle scale, simulated by CFD-DEM simulations and CFD/DNS (Direct Numerical) Simulations
- Intra-particle pore scale, simulated by Intra-Particle simulation coupled to CFD-DEM and
- Atomistic scale, simulated by Density Functional Theory (DFT) and Kinetic Monte-Carlo (MC) simulations

Porto serves to connect the different simulators, which is a non-homogenous set of in-house, open source – and proprietary simulators, running on different operating systems. The complexity and diversity of such a system requires that we have formal schemas and structures of meta-data that allows for information interpretation regardless of the original storage format and application. Porto offers the possibility to utilize MongoDB for meta-data and data storage, with features such as load balancing, data replication over multiple machines, map-reduce aggregation and complex searches.

The MoDeNa multi-scale simulation software framework

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Heinz Preisig
Norwegian University of Science and Technology, Trondheim, Norway

The MoDeNa project [1] aims at developing, demonstrating and assessing an easy-to-use multi-scale software framework application under an open-source licensing scheme that delivers models with feasible computational loads for process and product design of complex materials. The concept of MoDeNa is an interconnected multi-scale software framework. Four scales will be linked together by this framework namely the nano-, micro-, meso-, and macroscale (see Figure 1). As application cases we consider polyurethane foams (PU), which are excellent examples of a large turnover product produced in a variety of qualities and of which the properties are the result of designing and controlling the material structure on all levels of scale, from the molecule to the final product.

Multi-scale coupling requires the exchange of information between software instances developed for specific scales in a consistent way. In order to achieve this, generating consistent representations for models and data is necessary. The information exchange is governed by protocols and may occur in two ways, namely:

- "forward mapping" (passing information from the microscopic to the macroscopic scale in upward direction)
- "backward mapping" (passing information from the macroscopic to the microscopic scale in downward direction)

"Forward mapping" is relatively straightforward, while "backward mapping" inevitably requires iteration since changing the operating conditions at the fine level changes the feedback to the coarse level. "Backward mapping" can be realised by "two-way coupling" or by "fitting surrogate models". The first approach usually requires exchange of large amounts of data during runtime that may be expensive either due to the complexity of the data exchange or the computational cost associated with executing the microscopic-scale simulation. In such cases, replacing the microscopic-scale simulation with a surrogate model presents the only viable alternative. This operation inherently constitutes a transfer of data across scales and MoDeNa is unique in that it focuses on this approach.

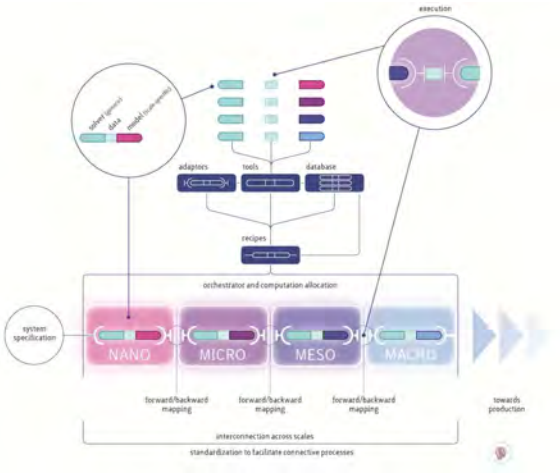

Figure 1: Conceptual structure of MoDeNa, coupling applications and surrogate models into tools, which form sequences through recipes and the orchestrator.

A typical operation sequence starts a macroscopic-scale simulation which instantiates one or more surrogate models. When the validity of a model is violated, a design of experiment operation is triggered. It creates inputs for a set of microscopic-scale simulations. When all experiments are finished, the parameter estimation component is invoked which updates the model parameters. Next, the macroscopic-scale simulation is restarted. It should be noted, that the MoDeNa software framework supports application and model dependencies across multiple scales.

The MoDeNa framework handles the communication across scales through recipes and adapters As shown in Figure [1]. Recipes perform simulations by executing applications (in-house codes or external software packages such as FOAM, Materials Studio, Predici) for a given set of inputs. Adapters handle the communication

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with the MoDeNa software framework. Both, recipes and adapters are application specific. Adapters exist as outgoing and incoming adapters. Outgoing adapters are relatively straight forward in that they perform a mapping operation (such as averaging) and communicate the results. The averaging process may have to be started and performed within the application (e.g. for time averaging). However, the results can usually be submitted in a separate process after the simulation is finished. Incoming adapters are more complicated since they usually require to embed surrogate models within the applications.

In this presentation the components of the MoDeNa software framework are described. The software framework consists of an orchestrator, a database and a interface library. The orchestrator is based on FireWorks [2] and constitutes the backbone of the software framework in that it schedules simulations as well as design of experiments & regression operations which make up the work-flow of the overall simulation. It is very much like a dynamic work-flow engine, in which the different applications are "orchestrated" to obtain information, analyse and pass it to the other operations. The NoSQL database MongoDB [3] is used to store the state of the work-flow as well as the surrogate models together with associated data such as model parameters, data used for regression analysis, and meta-data.

The interface library consists of two parts: A high-level python module providing access to the database as well as design of experiments and regression analysis capabilities by building on MongoEngine [4] and R [5], respectively. The second part is a low-level library providing unified access to the surrogate models. This component is written in C to ensure interoperability across platforms and target applications while providing the computationally efficient model execution required by the applications. The library is loaded as a shared library by the macroscopic-scale applications or as a native python extension by the high-level python module ensuring that all components instantiate identical model implementations. Complex operations such as database access are referred back to the high-level python module using call-back mechanisms.

References

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[2] Fireworks project web-site `http://pythonhosted.org/FireWorks/`

[3] MongoDB project web-site `http://www.mongodb.org/`

[4] MongoEngine project web-site `http://www.mongoengine.org/www.mongodb.org/`

[5] R project web-site `http://www.r-project.org/`

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Multi-scale modelling and simulations: a distributed and open-source platform approach

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Designed nanomaterials open up major opportunities for green technologies. The scientific challenge lies in understanding the material structure-property relationships. Computational modelling and simulations have become an indispensable and cost-effective tool in prediction of novel material properties and complementing experiments.

Nano-engineering is intrinsically strongly multi-disciplinary, which poses the organizational challenge to assemble the required expertise and resources. The advent of cloud computing and web-based modelling and simulations provided the opportunity to develop distributed computational approaches, thereby expanding and reinforcing the simulation capabilities enormously [1].

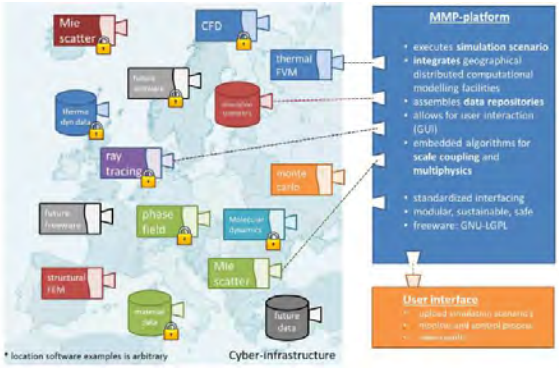


Figure 1: Schematic representation and vision of the integrating and distributed Multi-scale Modelling Platform (MMP) [2].

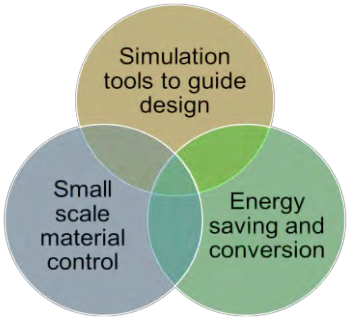
The MMP consortium has the ambition to develop an integrated Multi-scale Modelling Platform, especially equipped to target multi-physics engineering problems, see Figure 1. This allows integration of existing and distributed simulation software and data repositories as plug-in components.

A successful web-based framework needs to answer to the following requirements:

- **Standardized** data formats, communication protocols, simulation chain descriptions.
- **Secure** to protect companies IP.
- **Modular** for an extendible and sustainable platform architecture.

The predictive modelling of mid-power LED packages with remote phosphor is a challenging problem. Proper thermal management of such devices is critical to guarantee performance and reliability. However, the behaviour of phosphor-encapsulated dices is extremely difficult to predict, due to the absorption and spatial distribution of the heat generation.

This case study highlights the key aspect and capabilities of the integrated modelling approach. Moreover, it illustrates the type of data exchange and modelling linking which is required to address the typical multi-scale engineering problems.



Figuur 2: Main pillars driving the MMP ambition for: "smart design of nano-enabled products in green technologies".

Standardisation of data exchange and simulation processes is essential to achieve a sustainable and flexible platform design. Therefore, the MMP consortium is open to share and discuss the lessons learned and best practices in a wide modelling community.

References

[1] ICME: A Transformational Discipline for Improved Competitiveness and National Security, Nat. Research Council, USA, 2008.
[2] MMP, multiscale modelling platform: http://www.mmp-project.eu/

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Session 5: Integration Approaches and Techniques (chair A. Hashibon)

A. Cepellotti	**Invited talk**	AiiDA framework and integration
B. Patzák	**MMP**	On Design of MMP Multiscale Modelling Platform
H. Preisig	**MoDeNa**	Structured Ontology for Controlled Physical Processes

AiiDA: Automated Interactive Infrastructure and Database for Computational Science

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Computational science has seen in the last decades a spectacular rise in the scope, breadth, and depth of its efforts. Notwithstanding this prevalence and impact, very often simulations are performed without a consideration for the reproducibility, preservation, and sharing of the computational efforts. Great benefits could follow instead from adopting concepts and tools coming from computer science to design a "materials' informatics" infrastructure to automatically prepare, execute and monitor workflows of calculations for large classes of materials, and then retrieve and store the results in a format that can be easily browsed, queried and shared.

Our paradigm for such an infrastructure is based around the four "ADES" pillars of Automation, Data, Environment, and Sharing. I will here discuss the implementation of this paradigm in the open-source AiiDA platform (http://www.aiida.net [1]). The platform is tuned first to the demands of computational materials science. Transparent and extensible management of remote computational resources is obtained thanks to a machine-independent API for the interaction with remote computers and job schedulers, and allows for a tight coupling of automation and storage to ensure reproducibility. Provenance, preservation, and searchability of heterogeneous data are achieved through a design based on directed acyclic graphs with custom attributes. An embedded engine allows to encode complex sequences of low-level codes into scientific workflows to provide tested and shareable turnkey solutions for the calculation of material properties, boosting in this way the researchers' productivity.

By providing a flexible yet powerful infrastructure, we aim at providing the users with an intuitive high-level environment to access the advanced capabilities of the latest web/data tools, and at developing an ecosystem that encourages the sharing and dissemination of codes, data, and scientific workflows.

References

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On Design of MMP Multiscale Modelling Platform

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The reliable multiscale/multiphysics numerical modeling requires including all relevant physical phenomena along the process chain and across multiple scales, requiring the combination of knowledge from multiple fields. The development of a new multi-physics tool for a particular problem would be extremely time and resource consuming. A more viable approach lies in combining existing, usually single-physics tools, to build a customized multiphysics simulation chain for a particular problem. In order to achieve a full potential of such a modular approach, an integration framework is needed to provide underlying infrastructure that enables to facilitate data exchange and integrate/steer individual applications.

In this contribution, we describe the design of MuPIF platform [1], being developed in the frame of EU project Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies (MMP) [2]. The approach followed in this project is based on a application of object-oriented approach, consisting in designing a system of interacting objects. The abstract classes are designed to represent the entities in a model space, including, for example, simulation tools, fields, discretizations, properties, etc. The purpose of these abstract classes is to define a common interface to be implemented by each derived class and represented by a set of services that should be exclusively used to communicate with individual objects. Such interface concept allows using any derived class on a very abstract level, without being concerned with the implementation details of the individual components. The main feature is that individual applications as well as simulation data are represented by abstract classes. Therefore, the focus is on services provided by objects (object interfaces) and not on underlying data itself, leading to independence on particular data format(s).

The integration framework has been implemented in Python [1]. Python is an interpreted, interactive, object-oriented, multiplatform programming language. Such approach allows profiting from the capabilities of established scripting environment, including numerical libraries, serialization/persistence support, and remote communication. The complex simulation pipeline consists of top level script in Python language enriched by newly introduced classes. Later in the project, the top level script will be generated using a graphical tool.

Complex simulations are extremely resource and time demanding. Distributed and parallel computing environments provide needed resources and computational power. Common feature of these environments is a distributed data structure and concurrent processing on distributed processing nodes. This brings in an additional level of complexity that needs to be addressed in a platform design. The important role of the presented framework is to provide a communication mechanism that will take care of the network communication between the objects. The communication layer is based on transparent distributed object system fully integrated into Python. It takes care of the network communication between the objects when they are distributed over different machines on the network, hiding all socket programming details. This is achieved by the introduction of so-called proxies, a special kind of object that acts as if it were the actual object, forwarding the calls to the remote objects, and pass the results back to the calling code. An important feature, particularly for the end user, is transparency, hiding the details of remote communication to the user and allowing to manage local and remote objects using the same interface.

References

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Structured Ontology for Controlled Physical Processes

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Models are at the very beginning of model-based computational activities. Consequently, any error in models is beyond the most expensive ones and constructing models is a fundamental operation.

The effort we have since two decades is to construct models systematically based on the fundamental principles. Objective of the effort is to generate internally consistent models; models, that in our terminology are proper and convert the automatically into target code. The result of this research is a concise representation of physical models in the form of a block diagram. Based on this representation we have developed consecutively a set of programs that aid the user to generate these models as algebraic objects and translate them into computer code. The first commercial version has been established in 2003 being the foundation of a small company in the Netherlands. This realisation builds on a given set of equations representing each of the blocks in the basic diagram.

This first commercial version has a simple equation editor attached for entering the equations then to be used in the modelling process. Since then work has been going on to further systematise the approach and construct what we now refer to as ontology for such systems with the prospective for a further generalisation of the application domain and aiming at a standard for the model representation.

The concept of the ontology construction has been consolidated overt the past months and we have also established an interactive tool to generate and manipulate the ontology as a verification of the methodology. The ontology is coupled with a graph editor that allows for a hierarchical decomposition of a process and supports the generation of target code.

The presentation will discuss the fundamental ideas, and demonstrate briefly the use for generating the ontology for controlled physical processes. We shall indicate on how this approach will be used to model multi-scale processes, which is one of the avenues we will explore next.

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