Multiscale Simulation: from Materials through to Industrial Usage

5th – 7th September 2016

University College Dublin
O’Brien Centre for Science
Belfield, Dublin 4
Ireland
Foreword

Welcome to the CECAM Workshop on Multiscale Simulation: from Materials through to Industrial Usage. This is one of a series of workshops that have been organized jointly by 6 different EU supported projects and actions (DEEPEN, ICMEg, MMP, MoDeNa, NanoSim and SimPhoNy). The projects have the overarching goal to collaborate on developing data standards and interoperability interfaces to create integrated multi-scale modelling environments for nano-enabled materials.

This is the final workshop being organised by this cluster of projects. The workshop therefore builds on previous discussions regarding interoperability. It seeks to link together two different communities: multi-scale materials modelling (MMM) and those working in the area of Integrated Computational Materials Engineering (ICME). MMM focuses on the modelling of complex materials under realistic constraints in a wide range of situations. Almost all MMM discussions take a bottom-up approach, starting from ab-initio density functional theory and linking upwards via higher level models to predict key material properties at the micro- or nano-scale. From the other side, ICME starts from the application requirements, and aims to understand 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. ICME uses computational engineering as a major component aiming to remove the need for a lot of experimentation.

This workshop aims to bring together key speakers and groups that are addressing these challenges, to engage in practical discussions regarding what has been achieved to date and to roadmap the key steps to facilitate interoperability across the full spectrum of MMM and ICME applications.

One of the strengths of previous cluster workshops has been the time given to allow ample discussion of results. We want to maintain this atmosphere in Dublin, with a strong focus both on progress to date and routes to tackling ongoing challenges. We have therefore included two Panel discussions in the meeting, as well as including a combined poster and Plugfest session. The Plugfest is a particularly important part of the meeting, providing the opportunity for hands on overview, training and comparison of different platforms and linkage approaches. Each of the poster and Plugfest presenters is also invited to make a 2-minute presentation to highlight their key results. We hope overall for lively discussion and interchange in all sessions of the workshop.

The meeting is underpinned by sponsorship from the DEEPEN project, and also from Science Foundation Ireland. This has enabled us to provide travel support for invited speakers, as well as allowing us to set the workshop fees at a level to encourage wide participation.

We hope that you will enjoy the workshop and your visit to Dublin and Ireland!

Eoin O'Reilly (Conference Chair)
Workshop Scientific Steering Committee

Eoin O’Reilly (Chair),
Tyndall National Institute,
University College Cork, Ireland

Joan Adler,
Technion Haifa,
Institute of Technology, Israel

Shahriar Amini,
SINTEF, Norway

A.W.J (Sander) Gielen,
Technische Universiteit Eindhoven,
The Netherlands

Heinz A. Preisig,
Norwegian University of Science &
Technology, Norway

Local Organising Committee:

Kate Collins
Janine Galvin
Gerhard Goldbeck
Donal MacKernan
Eoin O’Reilly
Stefan Schulz
Programme Overview

Multiscale Simulation: from Materials through to Industrial Usage

The Workshop will take place at the O’Brien Centre for Science (Building 64 on map below), University College Dublin, Belfield from 5th to 7th September 2016.

The event will begin in Room H2.38 (Building 60, best entered through Building 64 and take the elevators (directly on your left as you enter the building) or take the round staircase (directly in front of you as you enter the building) to the second floor. At the top of the stairs go right (or from the elevator go left). Follow signs for “The Hub” and room H2.38 is the first left when you enter “The Hub”. There will be signposts to guide you.) with Session 1: Multiscale Current Status and Vision on Monday, 5th September. Session 2: Panel Discussions on Interoperability will close out the first day. An evening dinner will take place on the first evening at the Leopardstown Inn.

The second day will begin in Room H2.38 with Session 1: Current Developments and Challenges for Interoperability with developments from the cluster of five FP-7 funded projects, which are DEEPEN, MMP, MoDeNa, NanoSIM and SimPhoNY. Session 2 will be the poster session and Plugfest contributions, with hands on overview, training and comparison of different platforms and linkage approaches. Attendees presenting posters and Plugfest demonstrations will be given the opportunity to outline their work in a 2 minute oral presentation. This will be followed immediately by the poster and Plugfest session. The posters will be displayed for the first and second day of the Workshop. An evening dinner will take place on the second evening at the Brookwood Dublin Restaurant.

Day 3 will begin in Room E1.17 (Building 64) with Session 1: Roadmap, Future Plans and Directions for Integration, with invited and contributed talks. Session 2 will include a Panel selected from participants and will be a structured open discussion on future directions.

All refreshment breaks will be provided in the Pi Restaurant of the O’Brien Centre for Science building for all registered attendees on Monday, Tuesday and Wednesday.
Directions from Dublin Airport to Clayton Hotel Leopardstown:
Aircoach #700 goes directly from Dublin Airport to Clayton Hotel in Leopardstown. Note that Clayton Hotel was previously called Bewley’s Hotel; the hotel name has not been updated on the Aircoach leaflet
http://www.aircoach.ie/sites/default/files/dac/Dublin%20Map%20leaflet_0.pdf

Directions from Dublin Airport to University College Dublin:
Aircoach #700 also goes directly from Dublin Airport to University College Dublin, stopping on a slip road at the front entrance to the university
http://www.aircoach.ie/sites/default/files/dac/Dublin%20Map%20leaflet_0.pdf

Directions from Clayton Hotel Leopardstown to University College Dublin:
Organisers have secured taxis (two minibuses and a car) with the ‘NRC’ taxi company (‘NRC’ will be on the vehicle roof sign) to transfer attendees from Clayton Hotel Leopardstown to University College Dublin on each morning. The taxi journey is estimated 15-20 minutes, depending on traffic. Should you wish to travel by organised taxis, all vehicles will depart in front of the hotel at the following times:

- For Day 1, Sept 5th, taxi vehicles will depart Hotel for UCD at 08:45
- For Day 2, Sept 6th, taxi vehicles will depart Hotel for UCD at 08:45
- For Day 3, Sept 7th, taxi vehicles will depart Hotel for UCD at 09:00

Dublin Bus #47 (Bus stop in front of Clayton Hotel across the road) journeys to UCD (Get off at Stillorgan Road, UCD, stop 768). Note that buses are very infrequent in morning; there is a return bus every 30 minutes in early evening. https://www.dublinbus.ie/Your-Journey1/Timetables/All-Timetables/471/

Directions from Clayton Hotel Leopardstown to Leopardstown Inn:

15 minute walk down Brewery Road.
Directions from Clayton Hotel Leopardstown to Brookwood Restaurant:

Walk to Central Park/LUAS tram stop (about 350 m).
Take GREEN LUAS line to Stephen’s Green stop (terminus).
From Stephen’s Green stop, walk along north side of Stephen’s Green to Baggot Street:
Directions from University College Dublin to Brookwood Restaurant:

Walk to slip road at main entrance to university.

From there, you can get buses #39A, #46A and #145 to city centre.

#46A and #145: 600 m walk to restaurant from Lower Leeson St.

#39A: 160 m walk from Lower Pembroke St.
List of Taxi Companies

Lynk Taxis
Phone: (01) 471 53 33
www.lynk.ie

Ballsbridge Taxis
www.ballsbridgetaxis.ie
Phone: (01) 60 80 900

Trinity Taxis
www.trinitytaxis.ie
Phone: (01) 708 22 22

NRC
www.nrc.ie
Phone: (01) 677 22 22
Day 1 – 5th September 2016: Room H2.38

09:00 to 17:00 Registry
10:00 – 10:10 Joan Adler, Jim Greer Welcomes and Introduction

Session 1 – Multiscale Current Status and Vision
Session Chair: Adham Hashibon

10:10-10:50 Karsten Reuter (TU Munich) Frontiers in First-Principles Multiscale Catalysis Modeling
10:50- 11:10 Ellad Tadmor (University of Minnesota) Making interatomic potentials reliable and portable: the Knowledgebase of Interatomic Models (OpenKIM.org)
11:10-11:40 Coffee Break
11:40-12:00 James Warren (NIST) The Materials Genome Initiative and NIST
12:00-12:40 David Cebon (University of Cambridge) Multiscale simulation of materials in engineering industry
12:40-14:00 Lunch
14:00-14:40 Aidan P. Thompson (Sandia) LAMMPS: A general open-source framework for particle-based simulation of materials on multiple scales
14:40-15:20 Peter Deglmann (BASF) Polyurethanes - a challenge for multi-scale modelling
15:20-15:45 Tea Break

Session 2 – Panel Discussion on Interoperability
Session Chair: Pietro Asinari

15:45-15:50 Introduction
15:50-16:20 Georg J. Schmitz (Access e.V.) Towards Interoperability of Software Solutions in ICME settings
16:20-16:50 Adham Hashibon (Fraunhofer IWM) Towards a common template for materials data modelling and interoperability
16:50-17:50 Panel Discussion [with panel Claudia Draxl, Adham Hashibon, Georg Schmitz, Ellad Tadmor, James Warren]
19:30 Dinner, The Leopardstown Inn, Brewery Road, Stillorgan, Dublin 18
www.leopardstowninn.ie

Day 2 – 6th September 2016: Room H2.38

Session 1 – Current Developments and Challenges of Interoperability
Session Chair: Claudia Draxl

09:30-10:00 MMP Borek Patzak (Czech Technical University) Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies
10:00-10:30 MoDeNa Henrik Rusche (Wikki Ltd.) The MoDeNa multi-scale simulation software framework
10:30-11:00 DEEPEN Fabio Sacconi (TiberLAB) DEEPEN: interoperability for multiscale and multiphysics modeling of nanostructured devices
11:00-11:30 Coffee Break
11:30-12:00 SimPhoNy Adham Hashibon (Fraunhofer IWM) Interoperability Foundations in the SimPhoNy platform and its applications for multi-scale modelling

12:00-12:30 NanoSIM Jesper Friies (SINTEF) Multi-scale modelling using the Porto platform

12:30-12:45 Discussions

12:45-14:00 Lunch

Session 2 – Poster Session and Plugfest with hands on overview, training and comparison of different platforms and linkage approaches. The presenters of the posters and demonstrations will each be given 2 minutes for a brief overview of their work, followed immediately by the Plugfest and poster session.

Session Chair: Joan Adler

14:00-17:00 Poster session and Interactive Sessions

14:00-14:40 2 minute presentations on Poster presentations and on Plugfest contributions

Poster Presentations:

Po1. Jan Hamaekers (Fraunhofer SCAI) Localized Coulomb Descriptors for the Gaussian Approximation Potential

Po2. Borek Patzak (MMP) Multi-Physics Integration Framework MuPIF – design & operation

Po3. Erik E. Lorenz (Fraunhofer ENAS) A multiscale method for large-scale molecular dynamics simulations using off-lattice kinetic Monte Carlo events

Po4. Ian Thompson (University of Bath) Mesoscale simulations of a stacked organic light emitting diode

Po5. Omri Adler (SimPhoNy) Simulation and visualization with AViz - Nanotube vibrations

Po6. Ralph Altenfeld (MMP) Multiscale Modelling Platform (MMP) Implementing a CIGS Simulation Chain on the Mupif platform

Po7. Tobias Rasp (SimPhoNy) Investigation of fluid flow in a channel by coupling CFD and MD via SimPhoNy

Po8. Daniel Tanner (DEEPEN) Multiscale modelling of c-plane InGaN/GaN quantum wells: effect of random alloy fluctuations and structural inhomogeneities on the electronic properties

Po9. Mehdi Sadeghi (SimPhoNy) A P2P approach to run operations on distributed datasets

Plugfest Introduction:

PF1. **Punit Patel** (University of Warwick) Concurrent Multiscale Modelling of Materials Chemomechanics: an enabler for interoperable simulation codes

PF2. **Sigve Karolius** (MODENA) Model-based Design of Experiments in Multiscale Models

PF3. **Fidel Valega Mackenzie** (MMP) Multi-scale Modelling Platform (MMP): design of LED applications through distributed simulations

PF4. **Thomas Soini** (SCM, Amsterdam) ADF Modeling Suite: Easy scripting across computational chemistry codes

PF5. **Fabio Sacconi** (DEEPEN) TiberCAD and DEEPEN: tools for multiscale simulation of nanostructured devices

PF6. **Mehdi Sadeghi** (SimPhoNy) Hands-on demonstration of the SimPhoNy framework

PF7. **Georg J. Schmitz** (Access e.V.) MICRESS® – the MICRostructure Evolution Simulation Software

PF8. **Jesper Friis/Shahriar Amini** (NanoSIM) Multi-scale modelling using the Porto platform

PF9. **Joan Adler** (SimPhoNy) AViz - Atomistic Visualization

19:30 Dinner, Brookwood Dublin, 141 Baggot Street Lower, Dublin 2, www.brookwooddublin.com

**Day 3 – 7th September 2016: Room E1.17**

Session 1 – Roadmap; Future Plans and Directions for Integration
Session Chair: **Jim Greer**

09:40-09:45 Introduction
09:45-10:15 **Boris Kozinsky** (Bosch) Data informatics and provenance challenges in computational materials design
10:15-10:45 **Gerhard Klimeck** (Purdue University) NEMO5: Web Accessible Nanoelectronic Device Innovation with Multiphysics Atomistic Models
10:45-11:15 Coffee Break
11:15-11:45 **Claudia Draxl** (Humboldt University Berlin) From big data of materials science to scientific insight: the NOMAD Laboratory
11:45-12:15 **Judith Rommel** (Univ. of Cambridge) Predictive Multiscale Modelling in Chemical Sciences: Interdisciplinary Challenges from a Multidisciplinary View Point
12:15-12:45 **Heinz Preisig** (Norwegian University of Science and Technology) Multi-networks approach to multi-scale simulation
12:45-14:00 Lunch
**Session 2 – Panel Selected from Participants and Structured Open Discussion**

Session Chair: **Gerhard Goldbeck**

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Session 1

Monday, 5th September

10:10-15:45

Multiscale Current Status and Vision
Frontiers in First-Principles Multiscale Catalysis Modeling

Karsten Reuter

Chair for Theoretical Chemistry and Catalysis Research Center
Technische Universität München,
Lichtenbergstr. 4, D-85747 Garching (Germany)

As in many other areas of materials science, modern computational science is becoming a key contributor in the quest to quantitatively understand the molecular-level mechanisms underlying the macroscopic phenomena in chemical processing, which will ultimately enable a rational design of novel catalysts, energy suppliers and improved production strategies. Of particular relevance are hierarchical approaches that link the insights that modelling and simulation can provide across all relevant length and time scales. At the molecular level, first-principles electronic-structure calculations unravel the making and breaking of chemical bonds. At the mesoscopic scale, statistical simulations account for the interplay between all elementary processes involved in the catalytic cycle. At the macroscopic scale continuum theories yield the effect of heat and mass transfer, ultimately scaling up to a plant-wide simulation. A comprehensive control of catalytic and energy processes requires combining all of these facets and thus necessitates novel methodological approaches that integrate the various levels of theory into one multiscale simulation. In my talk I will review our recent activities in this field, focusing in particular on current challenges in the development of error-controlled first-principles kinetic models of complex reaction networks [1], as well as on the integration of such first-principles microkinetic models into macroscale computational fluid dynamics [2,3].

Making interatomic potentials reliable and portable:  
the Knowledgebase of Interatomic Models (OpenKIM.org)

Ellad B. Tadmor

University of Minnesota

Atomistic simulations using empirical interatomic models (potentials and force fields) play a key role in realistic scientific and industrial applications. This talk describes a US NSF-funded effort to develop an open-source online framework for facilitating the use and ensuring the reliability of interatomic models. The Open Knowledgebase of Interatomic Models (OpenKIM) (https://openkim.org) allows users to compare model predictions with reference data, to generate new predictions by uploading simulation test codes, and to download models conforming to an application programming interface (API) standard that has been developed in collaboration with the atomistic simulation community. Interatomic models are archived in OpenKIM with permanent citable IDs making it possible for others to reproduce published work. Models downloaded from OpenKIM can be seamlessly and directly used with any of a growing number of major simulation codes that support the KIM API. An overview will be given of the OpenKIM project and its main components which include the KIM API, the KIM data structure for representing arbitrary material properties, the KIM processing pipeline, the KIM visualization framework, and "RATE", a method for gauging model transferability.
In this talk I will present an overview of the US Materials Genome Initiative, and then focus on NIST’s efforts in support of the MGI. After an overview where I will provide insight into community-led activities, I will discuss our attempts at NIST to address some of the challenges to creating the materials innovation infrastructure that lies at the heart of the Materials Genome Initiative. In particular NIST is now devoting considerable effort, in concert with its partners in industry, academia and government, to develop the tools, standards and techniques for (i) establishing model and data exchange infrastructure (ii) establishing best practices and new methods for ensuring data and model quality and (iii) developing the data analytics to enable "data driven" materials science. Given the focus of the conference, I will tie these efforts into the essential role of the MGI data infrastructure in enabling multiscale materials simulation.
The grand challenge of materials modelling is accelerated development of new materials. Developing a new material for use in mission-critical situations, such as aerospace, defense and energy, can take 20 years or more. Shortening this time period requires a systematic approach: not only to material modeling, but also to the complex processes of material (and process) design, testing, validation and qualification. An arguably more manageable task is Integrated Computational Materials Engineering (ICME) which involves the integration of experimental and computational methods to understand the effects of composition, processing and structure on the properties of materials.

Most research into the materials development process has focused on methods for synthesizing the relevant material properties. This is itself hugely challenging, because material properties are controlled by structures/geometries over a wide range of length scales. Moduli, electrical and optical properties are controlled by structures at nanometer length scales: atomic bonding, atomic packing, atom sizes etc. matter here. Properties like strength and hardness are controlled at sub-micrometer length scales: dislocation movement, grain sizes, etc. are the key determining factors. Fatigue, fracture and wear properties are controlled by structures in the sub-millimeter range: flaws, microcracks, surface finish... In the majority of engineering applications, properties governed by behavior at all of these length scales need to be known before a material can be selected for use. So successful property synthesis for materials development would require validated multi-scale modeling approaches. These have not been developed for most classes of materials.

But multiscale modeling alone is not sufficient. Although it is possible to develop new materials without having a specific target application, this is unlikely to be a recipe for general success. The resulting material will only find a commercial use if, by chance, it happens to have a property profile that is particularly unusual and beneficial in some way. There are a few examples of such serendipitous success in materials development (for example polythene, pyro-ceram, warm superconduction), but the trail is littered with failed materials development projects: materials that may have shown some early promise, but have not yet found any large-scale application. Bulk amorphous metals, mechanically alloyed composites, and ceramic-matrix composites are all examples. This almost always occurred because the material was ultimately found not to provide the combination of properties - mechanical, electrical, thermal, processability, cost, etc. - needed to give sufficient benefit over the incumbent materials, to justify the cost and/or risk of change.

The alternative to hoping that a use will eventually be found for a new material is to treat materials development as a systematic design process. This involves defining the requirements (property profile) up-front; using systematic methods to propose promising
candidates (see figure); synthesizing their properties; simulating their behavior; optimizing their composition and structure, manufacturing samples and testing their performance.

Although software tools exist to support various parts of the materials design process: for example, predicting atom solubility or microstructures, calculating phase diagrams, etc., there is no existing methodology or software framework for combining these tools for the purposes of materials design.

This paper will propose a way forward for developing a methodology and tool set for use in materials design and ICME. At the heart is integrated access to material data: both experimental and synthesized. On top of this is layered a set of data interfaces and communication protocols that can be used to connect the necessary tools, so they can be used in concert. The result is a roadmap for research and development needed to enable systematic materials design across a broad range of material classes.
LAMMPS: A general open-source framework for particle-based simulation of materials on multiple scales

Aidan P. Thompson

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LAMMPS is a classical molecular dynamics code for simulating the dynamical behavior of large collections of particles. Originally conceived in the mid 1990s to run efficiently on the first massively parallel supercomputers, over time it has grown to become a large integrated package of methods and models. It is widely used in materials science and related fields to study how the atom-scale interactions in materials affect their behavior on larger scales. At the same time, LAMMPS implements a wide variety of physics models in which the particles represent something other than single atoms e.g. coarse-grained clusters of atoms, polymer beads, fluid particles, granular solid particles, and even electrons. In this talk, I will give an overview of LAMMPS' capabilities, with particular emphasis on applications involving advanced interatomic potentials and multiscale simulations. I will also discuss some of the disparate factors that have contributed to LAMMPS' success, including software design decisions, the evolution of computer hardware, the open source distribution model, as well as individual and organizational incentives.
Polyurethanes - a challenge for multi-scale modelling

Peter Deglmann

Quantum Chemistry
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The properties of polyurethane foams, an important large scale product, are the result of designing and controlling the material structure on all levels of scale, from the molecule to the final product. Polyurethanes are e.g. used in furniture, automotive, coatings, construction, thermal insulation and footwear. Tailoring their properties requires understanding and detailed modelling of the fundamental material behaviour on all scales.

For the example of this class of materials, the MoDeNa project aims at developing, demonstrating and assessing an easy-to-use multi-scale simulation toolbox with a GNU LGPL licensing scheme that delivers models with feasible computational loads for process and product design of complex materials. An open-source software-suite will be constructed that logically interlinks scale and problem specific software of university groups, using a software orchestrator that communicates information in both directions, namely upwards to higher scale and downwards to lower scale. This feature is unique, enabling the solution of complex material design problems.
Session 2

Monday, 5th September

15:45-17:50

Panel Discussion on Interoperability
Towards Interoperability of Software Solutions in ICME settings

G.J. Schmitz1*, A. Engstrom2, R. Bernhardt3, U. Prah14, L. Adam5, J. Seyfarth5, M. Apel1, C. Agelet de Saracibar6, P. Korzhavyi7, J. Ågren7 and B. Patzak8
ICMEg consortium: 1 Access e.V., Aachen, Germany; 2 Thermo-Calc Software AB, Stockholm, Sweden; 3 simufact engineering GmbH, Hamburg, Germany; 4 Steel Department of RWTH Aachen University, Aachen, Germany; 5 e-xstream engineering, Leuven, Belgium; 6 CIMNE Centre Internacional de Mètodes Numèrics a l'Enginyeria, Barcelona, Spain; 7 Royal Institute of Technology KTH Stockholm, Stockholm, Sweden; 8 Czech Technical University, Prague, Czech Republic, *corresponding author: G.J.Schmitz@micress.de

ICMEg – the Integrated Computational Materials Engineering expert group – a coordination activity of the European Commission launched in October 2013 and ending in September 2016 aims at developing a global and open standard for information exchange between the heterogeneous varieties of numerous simulation tools in ICME settings [1,2]. The ICMEg consortium [3] in cooperation with 5 other European projects on simulation platforms [4-8] has initiated and coordinated respective developments by a strategy of networking stakeholders during two “International Workshops on Software Solutions for ICME” held in 2014 [9] and 2016 (Barcelona) [10], by compiling identified and relevant software tools in a “Handbook of Software Solutions for ICME” to appear in autumn 2016 [11], by discussing strategies for interoperability between different software tools with all interested stakeholders, and eventually by compiling best practices towards interoperability and standardized information exchange in a White Book on interoperability [12]. The present contribution will shortly summarize these actions and present an overview of the current status and the insights gained during the project period. The presentation will especially address topics like highest level metadata categories [13] and ontologies [14], metadata descriptors for a system state [15], metadata schemata and namespaces, specific implementations of metadata schemata e.g. in HDF5 files [16] as well as others topics identified as being important for interoperability. The presentation will conclude with an outlook on future developments in these fields and also address the sustainable further continuation of the activities being launched by the ICMEg consortium e.g. within the European Materials Modelling Council EMMC [17] and the ICMEg association.

Acknowledgment
The research leading to these results has been performed within the ICMEg project and has received funding from the European Union Seventh Framework Programme (FP7/2007-2011) under grant agreement n° 6067114

References
[12] “White Book on interoperability”: interactive document summarizing status, learnings and perspectives in the area of interoperability of software codes. Copies of the actual version are available from the corresponding author
Towards a common template for materials data modelling and interoperability

Adham Hashibon

Fraunhofer Institute for Mechanics of Materials IWM, Woehlerstrasse 11, 79108 Freiburg, Germany & Board Member of the European Materials Modelling Council EMMC
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Advanced materials modelling for applications in industry requires a combination of various materials models that are used in linking and/or coupling workflows. As such, there is a need to move or transfer materials properties, data and models from one model and software tool to another in a seamless and efficient manner. There is a need to agree one vocabulary to both describe the models and their workflows.

Moreover, there is a need to curate the wealth of knowledge emanating from materials modelling, and of course experiments, in such a way that allows the proper collection, selection, archiving and retrieval of relevant information. Such curation of materials modelling data and seamless transfer of knowledge require a high level of interoperability to be established in order to bridge between the different semantic, terminologies and syntaxes used by different materials modelling communities (electronic, atomistic, mesoscopic and continuum). This information is to be translated into computational models and methods that can actually be used to run the simulations.

Semantic cross domain interoperability in materials data modelling in turn needs a specification of a complete and canonical metadata schema that is able to capture the structure, wealth and heterogeneity of data used to represent models and materials properties. This (meta-)data is composed of information, facts and knowledge on the computational representation of the material, specifically through materials models and how they are applied in a specific end user problem, the system that is modelled, its composition, size and geometry, etc., as well as how the materials model results are processed.

In order to devise such a schema, there is a need first to collect and establish a sufficient solid basis of knowledge covering all models and application scenarios that will later on enable the extraction of common ontologies, taxonomies and data structures. The challenge here is to collect all information covering all the different fields stemming from different modelling communities in a common way. A common template for materials data modelling and interoperability is therefore needed.

The development of such a template through the efforts within the European Commission DG R&I LEIT-NMBP, is to be found in the Review of Materials Modelling [3] and will be presented. It is shown that all basic elements of materials modelling can be represented in a four chapter organisation, the so-called MODA template [2]. Such a universal structure allows a more focused interpretation of modelling information and essentially provides a holistic view of materials modelling.

Metadata are discussed in the EMMC [3] and European Materials Modelling Cluster (EuMC) [4] and this enabled the development of a common universal data structures e-CUDS and common universal basic attributes (e-CUBA) that provide the basis for Semantic level interoperability of materials data that is independent of the implementation and provide a representation of the computational details of the MODA as a translation step of the end user problem into a simulation.

Session 1

Tuesday, 6th September

09:30-14:00

Current Developments and Challenges for Interoperability
Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies (MMP)


aCzech Technical University in Prague, bACCESS Materials&Processes, cCelSian Glass & Solar B.V., dVTT Technical Research Centre of Finland Ltd, eNetherlands Organisation for Applied Scientific Research TNO

A reliable multiscale/multiphysics numerical modeling requires including all relevant physical phenomena along the process chain, typically involving multiple scales, and the combination of knowledge from multiple fields. A pragmatic approach lies in combining existing tools, to build a customized multiphysics simulation chain. In order to achieve such a modular approach, a multi-physics integration framework MuPIF has been designed [1, 2] which provides an underlying infrastructure enabling high-level data exchange and steering of individual applications.

MuPIF is an object-oriented framework written in Python and built on abstract classes. The abstract classes define standardized abstract interfaces that allow to manipulate individual sub-models and high-level data components using the same generic interface. A top-level steering script orchestrates data exchange among tools and controls their runs. MuPIF supports a distributed simulation chain running on remote computers, taking advantage of secure communication, public/private key authentication, resource allocation, built on top of python remote object library Pyro4. This allows running MuPIF on various operating systems, arbitrary network setups while integrating in-house or commercial codes as independent entities.

A two simulation scenarios are developed in the MMP project [3], simulating a CIGS thin film growth process for the fabrication of solar cells and phosphors as light conversion material. The first scenario combines a CFD model, providing non-stationary temperature field on a furnace glass wafer and microstructure evolution model calculating the CIGS formation in a Cu-In-Ga thin film during selenisation by solving local phase distribution and element concentrations on a particular RVE. The second scenario combines optical model calculating the light absorption distribution inside the phosphor layer, blue die and the side walls of the molding component, which are transferred into the thermal model, where the absorption distribution is treated as an effective heat source. The thermal model calculates the stationary temperature distribution inside the entire LED and the transient temperature distribution during cooling down. Details of both scenarios will be provided on model coupling, their steering, distributed setup, performance and model outputs.

Finally, the current developments for achieving interoperability within a cluster and future challenges for the MuPIF platform will be presented and discussed.

The authors would like to acknowledge the support of EU FP7 project Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies (GA no: 604279).

REFERENCES
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.
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, PC-Saft) for a given set of inputs. Adapters handle the communication 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.

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 &parameter estimation 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 parameter estimation, and meta-data.

The interface library consists of two parts: A highlevel 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
DEEPEN: interoperability for multiscale and multiphysics modeling of nanostructured devices

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We present an Open Source software environment for the multiscale simulation of electronic and optoelectronic devices which has been developed in the framework of the FP7 Project “From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures” (DEEPEN) [1].

The aim of DEEPEN 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 nm CMOS. The software tools employed for multiscale simulations in this project have been integrated in the OS grid middleware environment UNICORE, by implementing suitable interfaces for the exchange of data and the coupling of simulations.

UNICORE is a general-purpose software suite providing access to compute resources as well as data resources. It follows the latest standards from the Grid and Web services world and offers a rich set of features to its users. UNICORE can be used in e-infrastructures of any nature and without limitations on the type of computing resource. Single PCs, cluster systems, or HPC systems are supported as well as different storage types. All UNICORE software is available as Open Source under BSD license from the UNICORE website [2].

An open source Common Data Format (CDF) has been defined during the project 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 [3]. Together with the CDF, the related input/output (I/O) application program interfaces (API), which provide 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. 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. HDF in general can be browsed like a unix filesystem, so that data to be exchanged in simulation workflows can be written in a hierarchical representation similar to a path. 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. Thus, 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 or for the implementation of a simple material parameters database. For example, the database parameters relevant to the project have been organized in groups in order to create a hierarchical structure taking into account the relations existing between them.

To implement the Open Source Interface (OSI) developed in Deepen in the framework of UNICORE system, two kinds of application software objects (GridBeans) for UNICORE have been developed for each tool involved in the workflows describing the multiscale simulation protocols. The first object, called Application Interface, is needed to handle the access to the tool in the UNICORE-based OSI. The second, the CDF Translator, is dedicated to the translation from the tool native file format to the CDF and vice versa. Fig.1 shows the overall schema of the OS multiscale environment implemented in the project. The simulation tools, such as OMEN, Wannier90, QE, etc. are given access to the OSI only through the Gridbean APIs and their respective translators available inside the Rich Client of the UNICORE environment. In this way, there is no need to modify the code of the single simulation tools to implement the APIs.

In case of a new version of a tool, only the Gridbean code must be updated, which may be performed even by the manager of the OSI platform, based on the tool public documentation. Similarly, data in the OSI are exchanged through the CDF translators, so that no information on the tool proprietary format is needed to link two different tools. In case of modification of the format of a tool, or when a new tool is included in the OSI, only the CDF translator for that tool must be updated, by the owner of the tool or, if format specifications are public, even by the manager of the OSI. In addition, since CDF is built on the OS HDF library, all the features of HDF APIs are available for I/O operations on data files and for the queries on the material database.

Finally, the workflows linking the simulation tools are implemented on the client/server UNICORE system in the following way. First, on the client side, the graphical editor allows to build each workflow in an interactive way (see Fig.2), while the Workflow services deal with the workflow and jobs execution. Then, on the server side, the submitted jobs are scheduled for execution through a queue manager called SGE that handles the requests and the hardware resources.

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References
Interoperability Foundations in the SimPhoNy platform and its applications for multi-scale modelling

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Advanced nano-enabled materials exhibit complex behaviour at all scales. Designing new materials requires that all materials properties and behaviour 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 where specific design and performance requirements have to be met. This essentially means that materials modelling workflows based on linking and coupling of various models each designed to describe a specific material behaviour have to be employed to obtain a reliable and predictive description of the material behaviour at all scales and consequently allow for an accelerated design of novel new materials.

Numerous models and tools exist that are able to describe a specific behaviour accurately and reliably using either electronic, atomistic, mesoscopic or continuum models. The FP7 EU project SimPhoNy [1] developed an open integrated materials modelling environment that integrates various existing disparate models and their respective simulation tools. The openness means here that the platform allows integrating both closed and open source applications on equal footings since the underlying integration system is based on open (meta-) data standards and APIs.

The main challenge tackled in SimPhoNy is to devise metadata and API specifications that are universally applicable to all models and related tools as well as to pre and post processing applications that span electronic, atomistic, mesoscopic and continuum models. In this presentation, the basic design of the SimPhoNy common unified data structure (CUDS) providing a metadata schema that provides a semantic interoperability layer and the common universal basic attributes (CUBA) that provide a cross domain syntactic interoperability layer will be presented. The main metadata schema is compatible and augmenting to the e-CUDS schema as described by the MODA [2]. The CUDS of SimPhoNy focuses on the translation of the MODA into the computational domain, giving a unified and interoperable (digital) representation of the material, the model equations, the boundaries and conditions as well as the computational numerical methods used. This enables moving data seamlessly between different tools regardless of the syntactic, domain specific data representation used.

Interface wrappers are developed for each tool that allow using existing materials modelling tools as plugins in the platform, whereby the wrappers implement the CUDS and CUBA to provide unified representation of the data and information throughout the different modelling tools. We shall demonstrate how this approach allows integrating electronic, atomistic, mesoscopic and continuum models to describe complex systems such as microfluidic flows in patterned channels by coupling atomistic molecular dynamics (MD) to continuum computational fluid dynamics (CFD) and complex fluids by coupling mesoscopic particle dynamics (using Discrete Elements Methods, DEM) to CFD.


Multi-scale modelling using the Porto platform
Within the NanoSim project, a non-homogeneous set of in-house, open source and proprietary software is connected in a multi-scale approach, enabling rational design of second generation gas-particle CO$_2$ Reforming technologies based on nano-materials. The final framework is sketched in Fig. 1. The complexity and diversity of this system requires formal schemas and meta-data structures that allows for information interpretation, regardless of the original storage format and application. Porto is an open data-centric lightweight and flexible platform for data and workflow management, developed in NanoSim to facilitate information flow and data sharing.

In this presentation, we will focus on the electronic and atomistic scale models of the NanoSim framework and show how they are interfaced to Porto. Density functional theory (DFT) is used to simulate the elementary steps of the chemical looping process on the haematite surface. The Vienna Ab-initio Simulation Package (VASP) [1,2] was used for the electronic calculations and to investigate the different reactions and adsorption structures. Fig. 2 shows schematically the different steps in hydrogen dissociation on haematite. Vibrational contributions are evaluated from postprocessing using the Phonopy package. [3]. A set of Python scripts via

![Figure 1. Flow of information between the different software tools at the end of the NanoSim project.](image1)

![Figure 2. Schematic for hydrogen dissociation on haematite.](image2)
new Python bindings were developed in order to extract parameters from these calculations and express them as *Porto* data entities for communication to higher-scale models [4].

These scripts read the input and output files of the *ab initio* calculations directly from (potentially complex) file system directory structures. We use the directory structure to express the relation between the different calculations, as shown in Fig. 3 for the $\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}$ reaction in the gas phase and on the haematite surface. One of the key design principles of *Porto*, is the separation of data (entities) and structures (relations). For this purpose, *Porto* defines *collections* as a special entity that contains information about other entities and relations between them. All relevant information from the input and output files is stored as Porto entities grouped together in a collection, where the ability of collections to express relations between entities is used to retain all the information implied by the directory structure.

Since the input is stored together with the output, the system will also be capable of reproducing the file system directory structure together with all input files. This is useful if one needs to redo or refine the calculations. The flexibility of the system makes it easy to extend the amount of information stored from these calculations.

References


*Figure 3:* Example of a file structure with VASP results. Relevant information from the files in green will be stored as Porto entities grouped
Session 2

Tuesday, 6th September

14:00-17:00

Poster Presentations and Plugfest Introductions
Localized Coulomb Descriptors for the Gaussian Approximation Potential

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We introduce a novel class of localized atomic environment representation functions, based upon the global Coulomb matrix, which have dimensionality either quadratic or linear in the number of atoms in the local atomic environment. By combining these functions with the Gaussian approximation potential, we present LC-GAP, a new system for generating atomic potentials through machine learning (ML). Tests on datasets demonstrate that potentials created with LC-GAP can successfully predict atomization energies for molecules larger than those used for training. Additionally, we show that LC-GAP provides accuracy comparable to and competitive with other ML-based potentials described in the literature. We further present our recent research results on the application of these descriptors for materials.
A reliable multiscale/multiphysics numerical modeling requires including all relevant physical phenomena along the process chain and across multiple scales, and the combination of knowledge from multiple fields. A pragmatic approach lies in combining existing, usually single-physics tools, to build a customized multiphysics simulation chain for a particular problem. In order to achieve such a modular approach, a multi-physics integration framework MuPIF has been designed [1,2] to provide an underlying infrastructure enabling high-level data exchange and steering of individual applications. MuPIF is an object-oriented framework written in Python and built on abstract classes. The abstract classes define abstract common interface allowing to manipulate and steer derived classes using the interface declared by the abstract parent class. One of the key features of the MuPIF platform is the definition of abstract interfaces for models as well as for high level data (representing, for example, spatial fields or microstructures). This allows to achieve true plug&play architecture, where individual application are manipulated using the same interface. As the same concept is applied for high level data, the platform can support different data formats, storage schemes and even data repositories.

MuPIF supports a distributed simulation chain running on remote computers, taking advantage of secure communication, public/private key authentication, resource allocation, built on top of python remote object library Pyro4. This allows running MuPIF on various operating systems, arbitrary network setup connections with firewalls while integrating in-house or commercial codes written using different languages. Recent simulation chains proved MuPIF capabilities on opto-thermal, CFD and phase thermodynamic models using softwares Matlab, Comsol, Xstream, Micress [3,4]. The distributed capabilities can be exploited in many ways, allowing to utilize HPC resources, or offering individual remote applications as a service.

MuPIF performance will be demonstrated on two open-source examples, see Figure 1. The first example solves a thermo-mechanical chain, coupling a 2D non-stationary heat conduction with an elastic material loaded by computed thermal strains. Resulting temperature and displacement fields are displayed using MuPIF’s support for VTK output. The second example solves a multiscale stationary heat transfer on a perforated ceramic sheet. Effective computed conductivity from a microscale is passed to a macroscale. Macroscale solves heat conduction yielding a temperature field.
MuPIF can be downloaded from its homepage [5] or through a standard Python's pip installer. In addition, the repository contains a reference manual, a user guide, the above-mentioned demonstration examples and other local and distributed examples. The authors would like to acknowledge the support of EU FP7 project Multiscale Modelling Platform: Smart design of nanoenabled products in green technologies (GA no: 604279).

REFERENCES
A multiscale method for large-scale molecular dynamics simulations using off-lattice kinetic Monte Carlo events

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The optimization of thin film growth processes is often supported by numerical simulations, which offer a wide variety of methods for different scales. The application of simulation methods for the reactor scale, feature scale and atomistic scale leads to a thorough understanding of the involved growth mechanics, although computational constraints limit each method to its own domain. By combining multiple methods into a multiscale method, the processes can be simulated efficiently on a large scale using a problem-specific simulation method.

In this work, a highly parallel multiscale method for the micrometer-scale atomistic simulation of thin film deposition processes is presented [1], which integrates kinetic monte carlo (KMC) simulations with molecular dynamics (MD) simulations. The presented method models individual arrival events during typical vapor deposition processes, such as physical vapor deposition (PVD), chemical vapor deposition (CVD) or atomic layer deposition (ALD). Each arrival event is modeled as an off-lattice KMC event, which is implemented through individual range-limited MD simulations (Fig. 1.). By highly parallelizing the KMC events while still retaining their temporal order, linear scalability can be achieved for surface areas up to 200 nm x 200 nm containing 107 atoms, while still supporting large simulation areas of 1 μm x 1 μm containing more than 109 atoms.

Computational efficiency is achieved by utilizing versatile data structures: Octrees are used for the efficient localization of KMC events and extraction of atoms in their local neighborhood. A fail-save, low/latency host-worker system enables efficient parallelization, for which mutual dependencies of overlapping KMC events are resolved using a directional multi-headed dependency tree. Structural analysis can be performed on the Delaunay triangulation of the bulk as well as the alpha shape, which represents the simulation surface.

The poster will give a short overview over the simulation method and its computational advantages compared to conventional MD and KMC methods. Physical vapor deposition (PVD) of gold on structured surfaces and of amorphous silicon is used to illustrate our approach. A direct comparison to pure MD methods is presented by the simulation of PVD of a copper-nickel multilayer system. A comparison of computational runtime measures with theoretical runtime models shows linear scalability up to a system-dependent limit. Interfaces for the linking to reactor scale simulations (computational fluid dynamics) and electronic scale simulations (density functional theory) are available. Reactor scale simulations can provide local process parameters (e.g. partial pressures, temperatures, particle energies) while gaining information about resource consumption, growth rates and surface morphology. Electronic calculations can provide the required interatomic force fields, reaction pathways and reaction kinetics for processes with complex chemistries. Reactive deposition processes (chemical vapor deposition, atomic layer deposition) can be enabled by preparing reactive force fields (ReaxFF).

Atomistically resolved structural models of the deposited films are the outcome of this approach. These structural models can be used to calculate material properties using
established procedures. Hence, the presented method provides an important step towards comprehensive simulations of thin film deposition processes, linking the properties of the grown materials to reactor conditions and vice versa.


![Figure 1](image1.png)  
**Figure 1** Coupling method for large-scale highly-parallel simulations in the presented simulation method: Off-lattice KMC surface site selection allows for range-limited MD simulations, which are run in parallel for improved efficiency.  

![Figure 2](image2.png)  
**Figure 2** Linking between different simulation scales: The presented method couples the Feature Scale and Atomistic Scale.
A 3-Dimensional mesoscale simulation has been undertaken of the electrical and optical characteristics of a stacked organic light emitting diode, OLED. Our Kinetic Monte Carlo approach adapted from organic solar cell simulations adds considerable capability to well established techniques of OLED simulation by allowing for interactions between the particle species, here electrons, holes, singlet and triplet excitons. We show that the materials composition and layer widths influence the recombination zone location and can significantly improve OLED output if materials and layer widths are chosen appropriately. If the recombination zone is narrowed, there is an improvement in the singlet generation yield via triplet-triplet reactions that can cause as much as an order of magnitude increase in the luminous efficiency. We examine the effects of changes caused by altering layer widths on the exciton formation efficiency and of outcoupling of light from the device which can compete. Both these effects are very sensitive to materials composition and geometry. Integration of the mesoscale simulation with microscopic simulations using the open source code BigDFT and with drift diffusion codes will be discussed.
Simulation and visualization with AViz - Nanotube vibrations

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One of the potential applications of the simulation and visualization techniques being developed in Sim-PhoNy is modelling a N(ano) E(lectro) M(echanical) S(ensor) to weigh molecules such as DNA, as shown in an idealised form in Figure 1. This would be attained by calculating the change in vibrational frequency when additional mass is attached to a vibrating nanotube. An image of such a nanotube, from the laboratory of Y. Yaish (reproduced from [1]) is shown in Figure 2. Proof of concept was provided by Pine et al [2] who changed the mass of the nanotube’s carbon atoms (by swapping for heavier isotopes) and showed that the resultant change in the vibrations of nanotubes reflected the additional mass.

The simulations of the vibrations were made with our own FORTRAN Molecular Dynamics using the Brenner [3] potential, to best take into account mechanical distortions while retaining simulation efficiency. The nanotubes were first equilibrated with periodic boundary conditions at 300 Kelvin and when the equilibrated length was found, they were frozen at the ends (equivalent to sitting on supports) and allowed to vibrate for an extended time to obtain sufficient data. The vibrational spectra were analyzed with Fourier transforms using our own MATLAB code to find the four lowest modes. The entire study included extensive investigation of nanotube type, boundary conditions and comparison with analytic models, [4, 5, 6]. Nanotubes with radii between 2.0 and 9.49 Å, having armchair, zig-zag and chiral structures were studied.

Of course, in order to weigh attached molecules, these need to remain adsorbed on the nanotube for the time needed for the vibrational measurements. Our initial adsorbed object was selected to be benzene. Our earliest attempts to study this system were plagued by benzene molecules flying off the nanotubes. Consultation with experimental students, from Y. Yaish’s laboratory, led to the suggestion that a flatter nanotube may lead to an extended period of adsorption. This was indeed the case, and successful simulations have been made and vibrational measurements have been taken.

After checking that the code as adapted to the wider nanotubes gave the same results when narrower ones were run with it, benzene molecules (minus their hydrogen atoms, which have little mass) were attached as shown in Figure 3. The images here are all from a (30,30), armchair nanotube with a radius of 20.46 Å and length of 184.45 Å. Two closeups, in anaglyphic stereo are shown in Figures 4 and 5. The stereo aids the 3-dimensional depth perception, and we selected colors that do not lead to color washout.

The vibrations for cases with benzene and other molecules in different positions, with both real carbon and heavier masses are being recorded and analyzed. Trends in vibrational modes are being studied and our poster will present details of these. Discussion and comparison with results of Yaish et al [9] will be included.
The nanotube structures and animations have been visualized with AViz[7, 8] at both the atomistic and electronic [11] scales, including analyglyphic stereo. The electronic scale modelling enables estimation of the nanotube width which is an important parameter for comparison with analytic models.

Acknowledgements: This study is part of the EUSimPhoNy project and relates to several of the use cases. O. Adler, thanks the SimPhoNy project for support. We thank P. Pine for advice in the initial stages, and Sharon Maliniak for discussions on nanotube radii.

References
In the frame of the MMP project [1], the partners TNO, CelSian Glass & Solar B.V., and Access e.V. are developing a simulation chain which models the fabrication of CIGS thin films in a selenization process. The simulation chain combines the macro scale process modelling, in particular the thermal conditions in the selenization furnace [2], with the micro scale thermodynamics and phase field models for the simulation of the phase formation in the precursor film (see figure 1). Besides the results of the individual simulations, a functional for the material quality ('quality factor') has been introduced which quantifies the thin film properties and helps the end user to evaluate the selenization process with respect to the fabrication of photovoltaic CIGS components [3].

![Figure 1 Schematic representation of the CIGS simulation chain](image)

This poster presentation focuses on the developed components which are necessary to implement and execute the simulation chain on the platform Mupif from the project partner CTU [4]. A top-level script controls the interaction between the interfaces of the participating...
simulation software packages, i.e. setting and getting parameter and data, initiating simulation steps, and post processing of the results for the end user. Enriched with preliminary results, the interplay of the components is shown.

Acknowledgment
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References
[1] www.mmp-project.eu: MMP project website
Investigation of fluid flow in a channel by coupling CFD and MD via SimPhoNy

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Simulating the behaviour of liquid flow through arbitrarily shaped channels on the macroscopic scale is a task that has been dealt with extensively in the past. Powerful Computational Fluid Dynamics (CFD) solvers based on continuum flow models like the Navier-Stokes equations have been developed, which can be applied to a wide range of liquid flow problems. The fluid flow in micro and especially nano-fluidic devices, which are e.g. required for bioengineering and chemistry applications, presents significant differences from the larger scale ones. In contrast to the macroscopic treatment, the no-slip boundary condition does no longer hold in nano-fluidic systems and the assumptions of the continuum approximations become inadequate at the solid-liquid interface.

A remedy to this issue is provided by Molecular Dynamics (MD) simulations, where the liquid is represented on a very small scale by the individual atoms or molecules composing the liquid. The trajectory of the atoms is determined by Brownian motion and the interaction with other atoms controlled by specific interatomic potentials. Therefore, a natural description of the flow/slip behaviour at the boundary, which can be represented by fixed atoms itself, is included in this method by design. MD simulations, however, are computationally more intensive than typical CFD systems and consequently only phenomena over relatively short time and length scales can be investigated. Thus, they are usually not applicable to describe the flow behaviour in the whole macroscopic channel over the whole time range of interest.

Multi-scale material modelling approaches have the ability to build a bridge between the two methods mentioned above and may help to solve the problem. Employing a heterogeneous multiscale method (HMM), the bulk of the liquid is still modelled by CFD, but the region of the liquid near the boundary is investigated in more detail by MD and the desired information is coupled back to the CFD model.

Developing such coupling and linking scenarios from scratch is a difficult and time consuming task. Open Simulation platforms (OSP) provide a novel approach to integrate existing state of the art computational modelling in a seamless manner. In this poster, the open simulation platform SimPhoNy is applied for running the individual simulations and realizing the coupling between both scales by transferring the requested data from CFD to MD and vice versa. SimPhoNy is well suited for coupling disparate simulations tools working at different length and time scales and provides standard schemas for input and output data of the individual solvers based on common unified data structures (CUDS), which provide a semantic and syntactic interoperability between different simulation engines, including also varying definitions of the applied methods. For the present problem, the fluid is modelled at the macro scale by the CFD SimPhoNy engine based on OpenFOAM® and at the atomistic scale by the MD SimPhoNy engine based on LAMMPS.
A simple example of a straight channel with Poiseuille flow velocity profile will be demonstrated. The CFD velocity field in the vicinity of the boundary is imposed as constraint on MD particles on the top boundary region inducing a Couette like flow profile (see image below). Similarly, the velocity field of atoms at a certain distance to the boundary is transferred back to the CFD solver after running the MD simulation for a number of time steps as a boundary condition to the macroscopic flow. 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 and the rheological properties of the MD fluid are calibrated to match the respective values of the macroscopic fluid phase.

Results of this coupling procedure are shown for a Lennard Jones type liquid in a very small nano-channel that can also be calculated by LAMMPS exclusively in order to compare the coupled solution with a single scale solution. Moreover, the method is 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 is investigated.
Multiscale modelling of c-plane InGaN/GaN quantum wells: effect of random alloy fluctuations and structural inhomogeneities on the electronic properties

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Over recent years, the III-nitrides, GaN, InN, AlN, and their respective alloys, have afforded the production of optoelectronic devices that emit bright light over a wide spectral range, including efficient emission in the previously unreachable blue spectral region [1]. Nitride-based semiconductors are thus already replacing the current inefficient incandescent and fluorescent household lighting sources, leading to great economic and ecological gains such as cheaper lighting and fewer greenhouse gas emissions [2]. The importance of this materials system was recognised with the conferral of the 2014 Nobel Prize in Physics on I. Asaki, H. Amano, and S. Nakamura for their work on nitride-based blue light emitting diodes.

In spite of the success of nitride-based devices, there remain aspects of the c-plane InGaN/GaN quantum wells of which they are made which are not fully understood. One such aspect is the remarkable coincidence in these devices of high defect densities with high efficiencies. This is vastly different from the characteristics of other III-V alloys, such as InGaAs. On the basis of evidence from experimental studies, this defect-insensitivity has been widely attributed to carrier localisation; under this description the carriers are localised to small regions of the quantum well such that they cannot diffuse to non-radiative recombination centres. This localisation has in turn been variously imputed to: random alloy effects, built-in field combined with well width fluctuations, gross indium clustering, or some combination of these. The aim of this theoretical study is to investigate the impact of random alloy fluctuations and structural inhomogeneities on the electronic properties of c-plane InGaN/GaN quantum wells.

The fact that micro-structural properties introduce carrier localisation effects which impact device properties means the modelling of these structures is a necessarily multiscale procedure. Density functional theory (DFT) alone would be too computationally expensive to treat device-scale effects, whilst continuum models would fail to account for atomistic effects. The semi-empirical models used in this work, loosely coupled to first principles calculations, are therefore ideally suited to model these systems, having both the computational efficacy to treat large systems and the precision to treat atom-scale effects. The full theoretical framework used comprises a local polarisation model, a valence force field model, and a tight-binding model. The coupling between these different elements of our theoretical framework is shown in Figure 1. The figure illustrates the first-principles foundation upon which the semi-empirical models are built, and subsequently fed into Schrodinger's equation. This is then solved for the single particle states, from which insights into localisation and other system properties can be extracted.

To achieve an atomistic description of realistically sized c-plane InGaN/GaN quantum well systems, we begin with Heyd-Scuseria-Ernzerhof (HSE) hybrid functional DFT calculations to extract key material parameters from small bulk supercells. For instance, elastic...
constants are calculated from our HSE-DFT data, and used to parameterise a valence force field model, based on that due to Martin [4], which can account for microscopic changes in strain over alloyed macroscopic systems. This is used to obtain the relaxed atomic positions in the alloyed supercells. The Berry Phase technique is then used to calculate piezoelectric polarisation coefficients upon which our local polarisation theory [3] is based. The Berry phase technique is also used to benchmark our local polarisation theory. An example is shown in Figure 2. Here, $\Delta P$ is the difference in polarisation between the equilibrium and distorted structures of a large number of randomly distorted CuPt-like InGaN cells. The dashed blue line indicates the case of perfect agreement between the Berry phase and local polarisation model. Finally, HSE-DFT is used to parameterise an sp$^3$ tight-binding model. The tight-binding model is benchmarked, for instance, against HSE-DFT data for the band gap bowing of InGaN alloys [5].

Our calculations reveal that random alloy fluctuations alone are sufficient to bring about carrier localisation effects in c-plane InGaN QWs. This result is important in the context of previous studies on nitride-based devices, where gross indium clustering was thought to be the source of carrier localisation, and shows that an atomistic approach is indeed necessary to capture critical aspects of the device physics. We find that these localisation effects are exhibited primarily by the hole states. When turning to the excited hole states we observe that localisation effects persist to of order 100 meV into the valence band, for as little as 10% indium in the quantum well, giving rise to a significant density of localised states. From a study of the modulus overlap of the wavefunctions, it is revealed that this localisation affects the states in such a way as to reduce the ease of carrier transport through the device. By investigating c-plane InGaN quantum wells over a range of indium contents, it is shown that localisation effects due to random alloy fluctuations increase with increasing indium content. An examination of the electron states shows that they are far less sensitive to the quantum well microstructure. However, the combination of electrostatic built-in field, alloy fluctuations, and structural inhomogeneities, such as well-width fluctuations, can nevertheless lead to significant localisation effects in the electron states, particularly at higher indium contents. The calculations also show that while the built-in field acts to separate the electrons and holes along the c-axis in InGaN quantum well structures studied here, the additional localisation due to the random alloy fluctuations leads to electrons and holes of varying lateral separation. This brings about the situation of individually localised electrons and holes, which accounts for the non-exponential decay transients measured in time-dependent photoluminescence (PL) experiments [7].

Overall, the work utilises a multiscale approach to offer a detailed and reliable atomistic description of the electronic properties of c-plane InGaN/GaN quantum wells.

A P2P approach to run operations on distributed datasets

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Coupling and linking in materials modelling requires moving often large data sets between different models. The application of each model may be executed on different network, which renders moving data inefficient. In this work we propose a collaborative solution to accomplish such operations. We distributed the workflow information and the login onto data producing and consuming machines.

The main idea here is distributing the operations instead of moving data-sets around. We show how we avoid moving data-sets unless it is absolutely necessary. We define and analyze a number of scenarios, which represent the most common scientific usecases. Then we demonstrate how we solve them in a decentralized network of collaborating peers. Moreover, we show how we break complex operation into simpler sub-operations. In addition, we show how we collect the results of those sub-operations to construct the main result.
Electron Transport in Mesoscopic Systems: TiMeS transport under UNICORE

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TiMeS (Transport in Mesoscopic Systems) is an open-source program to calculate either a Green's function (GF) or non-equilibrium Green's function (NEGF) for nanoscale systems for charge or phonon transport in nanoscale systems for Hamiltonians expressed in a localized basis to allow the partitioning of a system into reservoirs or 'electrodes' and a scattering region [1]. The three primary steps leading to a transport calculation with the TiMeS approach are: i) calculation of the surface Green's functions for the electrodes; ii) calculation of a Green's function for the entire system (electrodes and scattering region); iii) finding the scattering matrix from the Green's functions to enable calculation of the scattering wave functions across a region subject to open system boundary conditions.

The TiMeS transport simulator is 'Hamiltonian independent' in the sense it can be coupled to any programs that calculate electronic structure or phonon spectra; in the following the focus is on coupling to electronic structure Hamiltonians, specifically as calculated by density functional theory (DFT) programs, for the determination of charge transport. The interfaces currently are in place for TiMeS to couple to the following three DFT based electronic structure packages: OpenMX [2], DFTB+ [3], and Quantum Espresso [4]. Note that the latter is a plane-wave electronic structure based method, and to transform the resulting Hamiltonian matrix into a localized basis set requires the use of the intermediary program Wannier90 [5]. All of these program with the the exceptions of DFTB+ are open source codes.

The structure for the interface between OpenMX and TiMeS is illustrated in Fig. 1 and can be described briefly as follows:

- a self-consistent Hamiltonian and overlap matrices are extracted from an OpenMX DFT calculation
- TiMeS calculates a charge density matrix from the OpenMX data and as well introduces open system boundary conditions by calculation of electrode self-energies using a surface Green's function approach
- in case of the NEGF calculations this density matrix is returned to the DFT code to re-calculate the electron density and therefore updating the Hamiltonian matrix, this allows the output from the DFT code to become self-consistent with the open system boundary conditions imposed by TiMeS
- for either the GF (i.e. one-shot) or NEGF options, the transmission probability T(E) across the scattering region for an electron of energy E is returned
- from the electron transmission, current-voltage characteristics for the scattering region are returned based on the Landauer formalism

These steps have been implemented under UNICORE [6], an open source interface for distributed computing and data resources through a ready-to-run Grid interface. Unicore allows for 'Grid beans' and a graphical interface which allows for the coupling of different programs in a transparent method. Through the use of a common data format (CDF), programs translate their outputs into the CDF and as well the CDF files are converted into program specific data formats. Hence any codes can be readily coupled through use of the CDF's as only one application program interface (API) per program module need to be written.
A common issue with localised basis sets in electronic structures calculations is that systematic convergence with respect to the basis set size is difficult to achieve and to test. On the contrary, plane wave basis sets allow for systematic convergence with DFT calculations. To make use of the systematic convergence available from plane wave calculations for a TiMeS transport simulation, the Quantum Espresso DFT code [4] is coupled to the Wannier90 code [5]; the latter transforms a Hamiltonian expressed in a plane wave basis into a localized basis set of Wannier functions. The use of the intermediary transformation using Wannier90 is readily accomplished using the CDF as Quantum Espresso $\rightarrow$ Wannier90 $\rightarrow$ TiMeS. To demonstrate the functionality of the interface between both types of DFT code (localized and plane-wave basis sets) and TiMeS, the transmission for a silicon chain which is calculated with OpenMX-TiMeS as well with QE-TiMeS via Wannier90 code is illustrated in Fig. 3. The relative ease of coupling the different simulation tools combined with 1 the Unicore graphical interface for setting up calculations, allows for practical multi-scale calculations within a readily usable environment.

References
Concurrent Multiscale Modelling of Materials Chemomechanics: an enabler for interoperable simulation codes

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Fracture and creep are the dominant failure processes underlying many materials reliability issues. At the same time, fracture remains one of the most challenging ‘multi-scale’ modelling problems, requiring both an accurate description of the chemical processes occurring in the near tip region and the inclusion of a much larger region in the model systems. I will explain how these requirements can be met simultaneously by combining a quantum mechanical description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) approach such as the ‘Learn on the Fly’ (LOTF) scheme [1,2], implemented within the QUIP open simulation framework [3].

I will briefly present examples of the application of these techniques to ‘chemomechanical’ processes, where complex and interrelated chemical and mechanical processes that originate at the atomic scale go on to determine the mechanical behaviour of a material, e.g. interactions between moving cracks and material defects such as dislocations or impurities [4], or chemically activated fracture, where cracks advance under the concerted action of stress and corrosion by chemical species such as oxygen or water [5].

I will also demonstrate and discuss some of the methodology and tools developed to enable this work, e.g. the QUIP framework [3], the f90wrap package which promotes interoperability between codes by adding advanced Python scripting interfaces to existing Fortran packages [6], and an example showing how this can be used to exploit software tools such as CASTEP in new ways [7].

Software will be demonstrated from a standalone laptop using an interactive Jupyter notebook

References
3. https://libatoms.github.io

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Computer-based experiments have become a fast and inexpensive supplement to traditional physical experiments, typically used to guide development and experimental work. The traditional role of design of experiments (DoE) has been to select samples from the design space, the domain spanned by the input variables, according to a design criteria, for instance for the purpose of revealing measurement error. However, virtual experiments differ from physical because, although a computer simulation most certainly should be regarded as an experiment, there is a stark conceptual difference between the input-output relationship in a computer simulation and a real-world measurement. Simulation will, as discussed in [Santner et al., 2003], yield deterministic results for a given set of initial conditions; therefore, if a simulation is performed twice with the same set of parameters the computer produces identical results. Consequently, traditional experimental design techniques, which may focus on revealing measurement error through replication, will lead to an unnecessary amount of duplication when applied to a computer application due to the deterministic nature of the computational results.

This is of particular concern in a multiscale model, where the number of connections between scale-specific models increases rapidly; thus, the computational cost of the overall simulation quickly becomes impractical. The strategy for overcoming these practical challenges is to employ DoE and combining it with incorporate machine learning techniques and surrogate models, i.e. a simplified model mimicing the input-output behaviour of the detailed scale-specific models, that can be used in-place of computationally expensive simulations; thus, the speed of the simulation is increased without compromising accuracy, using a procedure commonly referred to as model-based design of experiments (MBDoE) [Franceschini and Macchietto, 2008]. There are various techniques for hybrid schemes that are based on the concept of replacing the direct coupling of two scales through a complex scale-specific with a simplified model. The so-called equation free approach [Kevrekidis et al., 2003] is a bottom-up perspective where the lower scale uses a surrogate model to fill-in information for regions where the complex model is not valid. Hierarchical multiscale modelling [Weinan et al., 2003] is a top-down method where parameters are replaced directly by a call to the surrogate model for the lower scale, as illustrated in Figure 1. In order to ensure that a surrogate model is always validated and MBDoE is an iterative procedure:

**Figure 1:** A multiscale model seen as a layered onion, surrogate models are employed to approximate the lower level scales.
The software framework developed in the project “Modelling of morphology development of micro and nanostructures” (MoDeNa) is designed specifically to facilitate scale coupling using surrogate models. In addition to addressing the recursive and parallel nature of traditional MBDoE, as described in [Galvanin et al., 2007], the framework expands the idea by performing the MBDoE when needed. This means that when the macroscopic scale in Figure 1, which employs a surrogate model of the mesoscopic scale, detects that the surrogate model is out of bounds or inaccurate it can request that the MoDeNa framework halts the main simulation and fixes the error.

Due to the fact that most single-scale models employ surrogate models of lower-level scales, potentially resulting in a chain reaction of MBDoE procedures illustrated in Figure 2, this inherently leads to an acyclic computational workflow. This is generally handled by employing workflow orchestrators, such as FireWorks [Jain et al.]. The MoDeNa framework embeds single-scale applications into the workflow management system and provides a library of strategies influencing how the MBDoE procedure is carried out. By facilitating embedding surrogate models as regular function calls, and at the same time be able to carry out MBDoE on-the-fly the MoDeNa software framework fills a lacuna in the library of multiscale modelling techniques.

References
Multi-scale Modelling Platform (MMP): design of LED applications through distributed simulations

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The high-tech industry strives to increase overall functionality and quality of products by the application of nano-enabled materials and devices. The development of such products significantly benefits from a thorough understanding of multi-scale and multi-physics phenomena and adequate numerical tools to guide nano-enabled design. Multiscale modelling and therewith multiscale design will considerably reduce development costs, decrease time to market and improve process yield and device functionality. These approaches contain scientific and organizational challenges:

- The main scientific challenge for building this platform lies in a proper definition of scale transitions and the associated information exchange between the relevant scales
- As nano-engineering is intrinsically strongly multidisciplinary, the expertise and simulation resources are distributed over different companies, research institutes, and academic groups.

The MMP project is developing an integrated modelling platform MuPIF (https://sourceforge.net/projects/mupif/), especially equipped to target multiscale and multi-physics engineering problems. The innovation of this platform lies in its generic, modular, and distributed concept, supported by data standardization and proper definition of application and data interfaces. This allows integration of simulation software, either academic, open source, or propriety, and data repositories as plug-in components, without any necessity to have all software in one computer or even in one network. This eases the cooperation between parties as no sensitive data or models need to be handed over, as well as development of the different (sub)models and simulation software can be handled independently.

Figure 1: Implemented nameserver+hub approach (left) used to run the simulation chain over different corporate networks. The black arrows represent the instantiation of connections, which is always from corporate network to outside, never reversed. The data flow will be bi-directional as soon as the connection is established. Geographical representation (right) of the network topology used during the platform integration test runs.
Although MuPIF can handle quite complex data streams and simulation control over multiple simulation servers, the IT security policies of companies in general prohibits these kind of complex connections. A key aspect of the IT security policies is that only out-bound connections are allowed. Therefore we implemented a nameserver+hub approach (Figure 1) to conform to the company IT security policies, but harnessing the power of MuPIF.

We will demonstrate the use of the models and platform in the current poster / presentation by assessing the performance of phosphor light conversion in LEDs in a distributed simulation chain. The opto-thermal simulation chain consists of four models: particle level scattering model, device level ray tracing model, and microstructural and device level thermal models. We will present particulars on the models and summarize the requirements for the application programming interfaces (API) to connect any software to the MuPIF platform. We intend to demonstrate the platform from the Plugfest location, using the simulation servers at VTT and TNO.

The main results of this project discussed here are two-fold: (1) We created a state-of-the-art simulation model for the opto-thermal behavior of LED’s, and (2) we can run the simulation chain over the internet, with direct and immediate data transfer between the different models, including remote control of the simulation chain.
ADF Modeling Suite: 
Easy scripting across computational chemistry codes

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An overview and demonstration of the scripting capabilities available for the molecular modeling codes in the ADF Modeling Suite [1] will be given. The typical accuracy and length/time scales that can be accessed with the different methods (molecular/periodic DFT, DFTB, ReaxFF, UFF) will be discussed. In addition, the available properties relevant for material science, in particular organic electronics [2], will be reviewed.

Besides the full integration of all the aforementioned codes within a single graphical interface, python scripting is also easy across the board, due to interfaces to ASE [3], PyADF [4] and PLAMS (Python Library for Automating Molecular Simulation) [5]. The 'Computational Chemistry Made Easy' project [6] builds upon PyADF and PLAMS, aiming to create an open source package dealing with more heterogeneous hardware, more quantum chemistry codes and including comprehensive workflow, data management and job management tools.

We will give a hands-on demonstration on how easy it is to set up the automation of repetitive though complex computational workflows involving the results obtained from different codes (ADF-based as well as external).

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[1] https://www.scm.com
[6] https://www.esciencecenter.nl/project/computational-chemistry-made-easy
DEEPEN environment for multiscale simulation of nanostructured devices

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We will present an Open Source software environment for the multiscale simulation of electronic and optoelectronic devices which has been developed in the framework of the FP7 Project “From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures” (DEEPEN).

The aim of DEEPEN 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 have been integrated in the OS grid middleware environment UNICORE, by implementing suitable interfaces for the exchange of data and the coupling of simulations.

We will see how the workflows linking the simulation tools are implemented on the client/server UNICORE system. First, on the client side, the graphical editor allows to build each workflow in an interactive way, while the Workflow services deal with the workflow and jobs execution. Then, on the server side, the submitted jobs are scheduled for execution on the selected computational resources.
Hands-on demonstration of the SimPhoNy framework

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The SimPhoNy project aims to develop an easy-to-use integrated multiscale modelling environment for *in Silico* discovery and design of nano-enabled systems and materials. The main concept of the SimPhoNy framework is to augment existing open-source and commercial simulation tools and supplement them with unified software interface wrappers and common data structures that allow seamless flow of information from one component to the other and from one model to another. The integrated tools cover electronic, atomistic, mesoscopic and continuum models and all scales from nano to the macroscopic device level scales.

The SimPhoNy framework moves the complexity of dealing with multiple third party simulation engines and pre/post processor tools to the application side. End users are able to interact with different simulation programs with one unified interface and a Common Universal Data Structure (CUDS). We show how the framework can be deployed and we demonstrate a number of simulations using various coupling and linking scenarios. In addition, we show how SimPhoNy can be extended by simply adding the necessary metadata components of the new models to the CUDS and developing the application based plugins to support the new tools. We further demonstrate how SimPhoNy allows for interoperability with other open simulation platforms.

SimPhoNy is an open source project and is available on [http://github.com/simphony](http://github.com/simphony)
MICRESS® – the MICRostructure Evolution Simulation Software

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MICRESS® - the MICRostructure Evolution Simulation Software – allows for the calculation of microstructure formation in metallurgical systems. The software is developed, maintained and distributed by ACCESS e.V., a non-profit research center at the RWTH Aachen University of Technology.

The evolution of a microstructure is governed by thermodynamic equilibria, diffusion and curvature. The strength of MICRESS® is the comprehensive treatment of these aspects.

MICRESS® applies a multiphase field method for multicomponent alloys and enables the treatment of multiphase, multigrain and multicomponent problems in the fields of solidification, grain growth, recrystallization or solid state phase transformations. All these phenomena can be addressed using this versatile and general tool. In the case of multicomponent alloys, the required thermodynamic data can either be provided in the form of locally linearized phase diagrams, or by direct coupling to thermodynamic data sets via a special TQ interface being developed in collaboration with Thermo-Calc AB, Stockholm. Commercially available thermodynamic and mobility datasets can be included for the simulation of microstructures in technical alloys like e.g. steels, superalloys, aluminium/magnesium alloys or solders.

The software covers phase evolution, solutal and thermal diffusion and transformation strain in solid state. 2D and 3D simulations are possible and the size of the simulation domain, the number of grains, phases and components are chiefly restricted by available memory size and CPU speed.

Additional models are available to tackle to stress/strain fields and their influence on microstructure evolution as well as a flow module allowing to study the effect of melt flow e.g. on dendrite growth. The homogenisation tool “HOMAT” allows the determination of effective properties of the materials from their microstructure and the knowledge of per phase properties. Recently a MICRESS® interface to the platform MuPIF (http://mech.fsv.cvut.cz/mupif) has been developed in the frame of the ongoing MMP project (Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies, http://mmp-project.eu, 2014-2016)

MICRESS® is currently installed in Europe, US, Japan, Korea, China, India and Australia at various customers from industry, governmental research centers and universities.

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Multi-scale modelling using the Porto platform

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Within the NanoSim project, a non-homogeneous set of in-house, open source and proprietary software is connected in a multi-scale approach, enabling rational design of second generation gas-particle CO₂ Reforming technologies based on nano-materials. The final framework is sketched in Fig. 1. The complexity and diversity of this system requires formal schemas and meta-data structures that allows for information interpretation, regardless of the original storage format and application. Porto is an open data-centric lightweight and flexible platform for data and workflow management, developed in NanoSim to facilitate information flow and data sharing.

In this presentation, we will focus on the electronic and atomistic scale models of the NanoSim framework and show how they are interfaced to Porto. Density functional theory (DFT) is used to simulate the elementary steps of the chemical looping process on the haematite surface. The Vienna Ab-initio Simulation Package (VASP) [1,2] was used for the electronic calculations and to investigate the different reactions and adsorption structures. Fig. 2 shows schematically the different steps in hydrogen dissociation on haematite. Vibrational contributions are evaluated from postprocessing using the Phonopy package. [3]. A set of Python scripts via

Figure 1. Flow of information between the different software tools at the end of the NanoSim project.

Figure 2. Schematic for hydrogen dissociation on haematite.
new Python bindings were developed in order to extract parameters from these calculations and express them as *Porto* data entities for communication to higher-scale models [4].

These scripts read the input and output files of the *ab initio* calculations directly from (potentially complex) file system directory structures. We use the directory structure to express the relation between the different calculations, as shown in Fig. 3 for the \( \text{CH}_4 \rightarrow \text{CH}_3 + \text{H} \) reaction in the gas phase and on the haematite surface. One of the key design principles of *Porto*, is the separation of data (entities) and structures (relations). For this purpose, *Porto* defines collections as a special entity that contains information about other entities and relations between them. All relevant information from the input and output files is stored as *Porto* entities grouped together in a collection, where the ability of collections to express relations between entities is used to retain all the information implied by the directory structure.

Since the input is stored together with the output, the system will also be capable of reproducing the file system directory structure together with all input files. This is useful if one needs to redo or refine the calculations. The flexibility of the system makes it easy to extend the amount of information stored from these calculations.

**References**


*Figure 3*: Example of a file structure with VASP results. Relevant information from the files in green will be stored as *Porto* entities grouped together in a collection.
AViz - Atomistic Visualization

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

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

Figure 3: Use of color to show defects (top) and layer mixing (bottom)
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. It is currently only available in LINUX, but in the framework of Sim PhoNy, the installation, from the files on Github [2] is straightforward. We will give demonstrations on an UBUNTU laptop, for data from a wide variety of models, including recent, not-yet published percolation applications.

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

**References**

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**Session 1**

**Wednesday, 7th September**

09:30-14:00
Roadmap; Future Plans and Directions for Integration
Data informatics and provenance challenges in computational materials design

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Design of new functional materials relying on transport phenomena is complicated by the highly nonlinear sensitivity of conductivity to structural and composition changes. This makes brute-force screening impossible and requires the development of descriptors and efficient approximations to narrow down the space of possibilities. I will briefly present our recent efforts on developing practical methods and data-driven approaches for the discovery and design of battery and thermoelectric materials. As is very common in the materials field, each investigation involves distinct scientific methods and data management specifications. At the same time, in each case there is a need to automate computational tools, organize and analyze the data, and preserve full record of data flow for reproducibility, while allowing for data sharing. The resulting workflows and data formats are heterogeneous and an automation platform is needed that is flexible enough to cover the common requirements and to leave the API interfaces open for implementation of specific scientific plug-ins by the users. The necessary features include tight coupling of data capture with automation, connecting computational engines in a high-level working environment, recording complete provenance information, and organizing data in an efficiently query-able form. Finally, data science tools are also needed for analyzing transport data, extracting and validating trends, to be used in iterative screening. A novel open-source software platform AiiDA (http://www.aiida.net) aims to satisfy the requirements by combining a Python automation engine with locally-deployed data management and analysis capabilities.
NEMO5: Web Accessible Nanoelectronic Device Innovation with Multiphysics Atomistic Models

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The technology road map brings new challenges to device designers. To achieve the goals such as high ON-current > 100 A/m, small SS < 60 mV/dec, the designs need to exploit new materials (III-V vs Si) and new effects (tunneling vs drift-diffusion current). In addition, the downscaling requires an atomistic treatment of the device that consists of 1M-100M atoms even at ultra scale. That's why only a multiscale approach is usable for modeling of new transistor designs. NEMO5’s aim is to provide multiscale high performance simulations for users, both locally or through the web [1].

NEMO5’s capabilities are as follows: valence force strain model, band structure calculations with different models (effective mass, k.p, empirical tight binding), electrostatics analysis with nonlinear Poisson equation on different scales, and quantum transport simulations with different approximations, such as ballistic transmission, quantum noncoherent transport with and without energy dissipation. Those models can be combined in a multiscale way allowing, for example, coupling between locally thermalized device areas (highly doped leads) to the regions where scattering may be neglected (e.g. MOSFET short channel < 15 nm) as shown in Fig. 1. NEMO5 allows for the creation of a model composed of any crystalline material and disordered systems. Imperfections such as surface roughness, random alloy and doping can be modeled.

Another multiscale feature of NEMO5 is the ability to import data from the simulators that work on a different scale. When working with a new material with (almost) unknown band properties, the first step is to simulate its unit cell ab initio. The ab initio results are mapped to the tightbinding model [2] to enable modeling of an electron transport in NEMO5 as shown in Fig. 2. If this approach is still too resource demanding, NEMO5 supports low rank approximations methods that can reduce simulation time [3,4]. On the other hand, the device structure has to be simulated on a very large scale in order to know where the atoms are under strain condition that occur. This can be done either in NEMO5 using the empirical VFF model, or molecular dynamics simulations from other codes [5].

NEMO5 scales to over 200,000 cores and can take advantage of Xeon Phi and GPUs. NEMO5 is extendable via user-defined Python scripts and a GUI allows for collaborative interactive device design. Additionally, a set of templates is available for typical devices such as nanowires and UTBs. NEMO5 is free to use for non-commercial purposes and has a distribution and support group on nanoHUB.org. Specific device simulations are available through nanoHUB.org tools, such as Quantum Dot Lab, Band Structure Lab, RTDNEGF, and NEMO5 simulations can be run through a web browser in nanoHUB’s workspace [6].

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Fig. 1. DGMOSFET with In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Al$_{0.48}$As superlattice with 3 InGaAs wells and 4 InAlAs barriers. Energy resolved densities for a) equilibrium boundary set at x=15nm (in the source) b) equilibrium boundary set at x=35nm (beside the channel) c) in the spacer region when the left equilibrium boundary is at x=35nm (beside the channel) and x=15nm (in the source). d) Transfer characteristics with VDS=0.3V and Ioff=0.1A/m. Dashed red line shows 60 mV/dec.

Fig. 2 a) Grain boundaries were generated in a copper nanowire of 3x3nm 2 cross section and 30nm length and were relaxed by MD b) Extended Hückel (EH) parameters were obtained by fitting EK diagrams obtained from abinitio simulations c) Transmission result for copper wire calculated by NEGF.
From big data of materials science to scientific insight: the NOMAD Laboratory

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On the steady search for advanced materials with tailored properties and novel functions, high-throughput screening has become 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 reliable methodologies to accurately describe all relevant properties for all materials on the same footing, and new concepts for getting insight into the materials data that are produced since many years with an exponential growth rate.

What are our concepts for tackling big data of materials science? It is not an issue of boosting more high-throughput calculations but it is about the question: *How to exploit the wealth of information, inherently inside the materials data which promises unprecedented insight?*

I will first introduce the *NoMaD Repository* [1], which was established to promote the idea of open access and sharing of materials data. 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. The latter is now being realized in the Novel Materials Discovery Laboratory – a European Center of Excellence [2]. Here the main aims are the creation of a *Materials Encyclopedia* and the development of big-data analytics tools for materials science. Finally, I will demonstrate some examples how statistical-learning approaches based on domain-specific knowledge can indeed lead to new scientific insight [3].

[2] NOMAD Center of Excellence, funded by the EU within HORIZON2020: http://nomad-CoE.eu
Predictive Multiscale Modelling in Chemical Sciences: 
Interdisciplinary Challenges from a Multidisciplinary View Point

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At the moment we see a rapid development of computers and simulation techniques. In 10 years’ time many chemists will first model their experiments computationally before implementing them at the bench to use existing knowledge and to predict the unknown. Seven interdisciplinary challenges we will have to overcome to bring computational chemical modelling closer to predictive molecular engineering and in silico design of new materials and drugs have been identified in a recent review.(1) We will relate these challenges to our improvements of the embedded atom method, one of which is the conscious inclusion of parametric uncertainties in the modelling process.(2) Additionally, we will highlight our latest advances in multi-scale simulations of chemical kinetics of self-assembling Glycine molecules on Cu110. We found substantial energy barriers for the diffusion of Glycine molecules parallel or across the Cu110 steps.(3) In future, the interplay of physical chemistry with other scientific disciplines such as mathematics, engineering, and visualisation science will lead to an inclusion of targeted molecular systems engineering research environments into the field, where predictive simulations enhance developments cycles, reduce costs and risks, and generate new ideas for experiments to design new drugs or materials and maybe one day allow for the virtual testing and design of a whole airplane.

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Multi-networks approach to multi-scale simulation

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Multi-network approach

Materials are not homogeneous but have distinct domains, crystals, zones, layers, or the like. Processes are typically performed in more than just one unit. Thus if one views the physical object then it is seen as having a granular structure of one or the other type. If one looks into smaller scale, then the granular units get smaller and smaller as one zooms in more and more.

The granular nature is thus the common part – granulates that interact with each other and are embedded in an environment that affects their behaviour. The underlying structure is thus a network of active granulates and interactions between them. Abstracted, this maps into a directed graph, where the granulates are captured by the nodes/vertices and the communications by arcs/edges and capturing materials on different scales thus implies hierarchical graphs or networks of networks.

Ontology-driven approach

MoDeNa (Development of an integrated multi-scale modelling environment for nano-materials and systems by design) defines the need for generating software containers, which for the models lead to an extension towards an ontology-driven approach. Consequently a new project has been started extending the model representation beyond MoDeNa: The definition of the ontology goes in steps building the mathematical representation recursively adding a list of variables and equations. The systematic approach to the construction of the equations ensures that the equation/variable system is structurally sound. Allowing for multiple equations describing the same phenomenon captures multiplicity of possible applications.

Model generation

The model for a particular material or process, for that matter, is established by defining the networks as it is seen by the person modelling the particular process in terms of capacities and transfer of extensive quantity between the capacities on the relevant scales. Connection between the scales is done by selecting mathematical models for the two actions of transferring information from the larger to the smaller scale model and vice versa. The terminology for the two operations varies from community to community but in the world of molecular dynamics it is often referred to lifting and homogenisation.

This process will extract the equations from the base ontology and add a lists of index lists, which refer to what equation is used for what node or arc and for what particular chemical / biological species or energy in one or the other form. Adding instantiations of the involved boundary and initial conditions as well as all involved parameters and constants, the model is complete.

Utilisation
Once the model is instantiated, meaning model equations have been selected, model networks are defined including the communication paths between the networks and all numerical information has been given, the equations can be compiled into the target computer language. Adding the solver and the necessary infrastructure generates a simulation for the application.

The approach makes it easy to choose for different target environments. The small compiler can be readily adjusted to generate alternative target code and with the file format being text with a simple schema definition as their definition, processing the information is readily done.

**Conclusions**

The chosen multi-network structure is now able to capture any level of complexity: On the same scale the network can capture complexity of the structure, such as discretised spatial representations of physical systems. It can capture interactions of materials/processes on the same scale but of very different nature, such as different phases or processes augmented with control equipment. It can capture multi-scale processes where the intra-network connections provide the vehicle to bridge the scales.

The structures are build on a minimum of meta terms and thus easy to implement and use. A new version of the ontology editor is operational.

The language to capture the equations is simple and requires minimal resources for the construction of an appropriate compiler.

Definition of variables and equations is now clearly separated from the utilisation, which opens the doors for a more wide use of the mathematical models capture in the ontologies.

Automatic compilation combined with a software factory enables the efficient generation of stand-alone applications.

The implemented approach has the potential to serve as a common platform for storing context-dependent models in a common repository.

**Associated publications**

- Preisig, H. A. Constructing an ontology for physical-chemical processes Computer-Aided Chemical Engineering, 2015, 37, 1001-1006
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Future plans for integration envisioned by the European Materials Modelling Council (EMMC)

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The gap between fundamental research and successful industrial innovation is commonly called the innovation valley of death. Bridging this valley quite often calls for tailored materials to be developed as fast as possible and this is the point where modelling and simulation can make a difference. Building this bridge calls for a focus of R&D efforts on industrial value chains, ranging from raw materials over materials to components and ends up in products.

Within industrial value chains, Computer Aided Engineering (CAE) is today widely used at a component level, mainly by continuum models for structural mechanics and process fluid dynamics, or on system level using flow chart simulators. These tools are successfully used for example in the automotive and in the chemical industry. The next generation of CAE tools are expected to extend these capabilities by including discrete models as well (electronic, atomistic and mesoscopic), which are a particular strength of the European research landscape, upstream the value chain to Computer Aided Materials Engineering (CAME).

The European Materials Modelling Council EMMC (http://emmc.info) has been set up in a bottom up fashion exactly in order to fully unlock the potential of Materials Modelling in industry. The approach of the EMMC is to start from industrial challenges by modelling of Key Performance Indicators (KPI) based on experimental data repositories and interoperability of predictive Materials Modelling software tools. Decision Support Systems will integrate the KPI modelling and interpolate the information gathered from experiment and simulation in order to identify the set of best compromises between KPI’s and business related cost measures.

Among other activities, the EMMC promotes wide European stakeholder consultations (last one done on May 2016), in order to define future plans for materials modelling integration and exploitation in industry. The plans are usually formulated in terms of Road Maps, which can be refined by further comments of the stakeholders. These Road Maps are then forwarded to the European Commission for possible consideration in promoting materials modelling in Europe.
Delivering on the promises of high-throughput atomistic simulations using verification, data provenance and workflows

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Abstract

The last decade has seen a clear shift in computational materials science towards establishing high-throughput approaches as a cornerstone of materials discovery and understanding. The community has developed a litany of tools, databases, protocols, jargon, etc. often borrowing from other fields that were earlier to undergo such a transformation. Within MARVEL (a pan-Swiss centre of research competence) we adopt a hierarchical approach that can be roughly split into three tiers. At the bottom are the atomic simulation codes, usually (though not exclusively) electronic structure theory. The middle tier consists of a database-driven, provenance tracking and automation engine that unifies the submission of calculations across different codes and computational resources while keeping track of the full provenance of any result, thus enabling full reproducibility. The last tier consists of an easy to use, yet powerful, workflow engine that allows experts to encode their knowledge and decision making to automate common tasks and make sophisticated calculations accessible to non-experts. These final two tiers are implemented in the AiiDA Python platform.

To demonstrate the enabling potential of such a platform I will discuss two examples. One revolves around providing data on demand services to researchers without sufficient expertise or computational resources as part of the MaX H2020 project. The goal here is to take non-domain experts from a crystal structure or other input data all the way to properties with minimal to no intervention by us. The other aims to broaden our knowledge of low-lying binary crystal structures by filling in the gaps in the PAULING FILE, an extensive database of experimental structures and properties. Neither of these two would be possible without extensive verification of the reliability, robustness and accuracy of each tier of our platform, some of which will be highlighted.