Communication Standards and Open Simulation Platform

NMP project cluster

The EC NMP Programme launched two Calls in 2011 on multi-scale modelling and started 5+1 projects. The projects should (among others) “facilitate a harmonised approach”, and in particular “interact on the definition of software interfaces, and the development of inter-process, and inter-scale communication.”
The five Collaborative Projects DEEPEN, MMP, MODENA, NANOSIM and SIMPHONY work on the definition of software interfaces, and the development of inter-process, and inter-scale communication. The project ICMEg (Integrated Computational Materials Engineering expert group) is a networking project (CSA) aiming to facilitate and develop an open and easily accessible formulation of a global standard for information exchange in ICME. A description of muti-scale modelling activities in several of the projects is appended.

The 5+1 projects have agreed to cooperate in a cluster to work out proposals for meta-data and data structures for file based information exchange. The communications standards will be based on existing standards to the largest possible extend. They will allow sequential i.e. file based interoperability between different software packages. In particular, the 5+1 projects have agreed to collaborate on the following tasks:

Communication Standards

a. **Generic and structured list of metadata keywords and an Alias Table for keywords describing the same metadata.**
b. **Overall data structure for file based information exchange.**

Each project will make their own platform adhering to these standards.

The 5 collaborative projects will run interoperability workshops and ICMEg will organise open workshops to get wide endorsement of these proposals and promote the use of standardized nomenclature.

The targeted timeline for the cluster is:

- June 2015: Public cluster proposal for metadata keyword list published on the ICMEg project and EMMC websites for wide discussion
- Dec 2015: Public cluster proposal for a file data structure
- Dec 2015: Public Cluster proposal for platform (linking, single computer)
- Dec 2017: Public Cluster proposal for platform (coupling, distributed)

EMMC

These NMP project actions will be complemented by the EMMC in the Interoperability Work Group. This EMMC Work Group will involve all players who want to participate actively in the determination of communication standards and interoperability. There is the hope that in the not-too-far-future Europe will be working with widely accepted, thus de-facto standards.

The EMMC recommends to the EC to support the development of an open simulation platform based on these standards which could be used to link and couple all existing materials models, as follows;

Open Simulation Platform

a. **Workflow tool(s) to orchestrate a number of different materials modelling tools (see Review of Materials Modelling for the scope of these tools); on one computer; first for linking than for coupling of simulations.**
b. **Tools for distributed simulations.**
c. **Accounting schemes (not for the use of the platform but for the use of commercial codes used in the platform operation by the user e.g. SME).**

Modelling in SimPhoNy 604005

Subject of the modelling

Integrated multiscale modelling environment applied to nano- and micro-fluidic applications

Physics/Chemistry models used

Electronic:	Density Functional Theory (DFT)
Atomistic:	Molecular Dynamics (MD)
Mesoscopic:	Coarse-Grained Molecular Dynamics (CGMD), Dissipative Particle Dynamics (DPD), Lattice Boltzmann (LB)
Continuum:	CFD solved by FVM and FEM, Smoothed Particle Hydrodynamics (SPH) and Particle Dynamics methods (DEM)

Simulation software and type of numeric used

Electronic:	Quantum-Espresso and VASP (DFT)
Atomistic:	LAMMPS (MD)
Mesoscopic:	LAMMPS (CGMD and DPD), JYU-LBM and Palabos (Lattice Boltzmann Methods)
Continuum:	OpenFOAM (FVM), NUMEROLA (FEM), Kratos (FEM, DEM), SimPARTIX (DEM, SPH), LIGGGHTS (DEM)

Achievements of the model beyond experiments

The applications developed in the SimPhoNy project will enable scientists and engineers to obtain information that current experimental technology is unable to reveal easily, such as molecular structure and thermodynamics properties in the liquid near walls or in confined regions and self-organization of nanoparticles and fibers as a function of local fluid properties.

Application

- Nanotubes as single molecule-mass detectors or NEMS (Nano-Electro-Mechanical Systems)
- Optimization and design of novel nano-printing processes
- New foam-forming process for biodegradable materials
- Enhanced nano- and microfluidics

Relevant review articles covering the topic (not necessarily their own):

1. E. Weinan, B. Engquist, X. Li3, W. Ren, E. V. Eijnden. Heterogeneous Multiscale Methods: A Review. Commun. Comput. Phys., 2, 367 (2007).
2. J. Larson, R. Jacob, E. Ong. The Model Coupling Toolkit: A New Fortran90 Toolkit for Building Multiphysics Parallel Coupled Models. Int. J. High Perf. Comp. App., 19, 277 (2005).
3. S. Portegies Zwart, S. McMillan, at al. A Multiphysics and Multiscale Software Environment for Modeling Astrophysical Systems, New Astronomy, 14, 369 (2009).
4. J. Hegewald, M. Krafczyk, at al.. An agent-based coupling platform for complex automata. ICCS, volume 5102 of Lecture Notes in Computer Science, Springer, 227, (2008).
5. M.J. Buehler, J. Dodson, J., Meulbroek, P., Duin, A. & Goddard, W. A. The Computational Materials Design Facility (CMDF): A powerful framework for multiparadigm multi-scale simulations. Mat. Res. Soc. Proceedings, 894, LL3.8 (2006).

Summary of project

SimPhoNy will develop data interoperability interfaces that allow seamless linking and coupling of models each describing material phenomena on a specific scale. These models will be the building blocks for multiscale simulations. One of the main focuses of the SimPhoNy project is to develop a user friendly, extendable and open platform for the integration of various existing open source and commercial simulation and pre- and post-processing software packages. Integration will be facilitated by wrapping the simulation packages by an efficient interoperability interface designed and implemented in a high level language, namely Python, with a common application programming interface (API) to the outside world. The system will allow both linking (sequential execution) and coupling (concurrent execution) of codes. The SimPhoNy consortium also tackles fundamental questions pertaining to linking and coupling of models, namely filtering and loss of information between models and continuity and reversibility of information across models applied to different scales. From

the application side, SimPhoNy focuses on a cluster of related nano- and microfluidic applications that requires solving of problems not addressable by individual codes alone.

Standard interfaces and data structures

The SimPhoNy Application Programming Interface (API) provides a common interface to all simulation software tools, while the data compatibility layers, using the Common Universal/Unified Data Structure (CUDS), take care of data conversion between the different computational and pre- and post-processing tools and the SimPhoNy environment. Together with 5 other NMP projects on multi-scale modelling (DEEPEN, ICMEg, MMP, MODENA, and NANOSIM) communication standards (metadata keywords and an overall data structure for file based information exchange) will be elaborated. These will be used in the SimPhoNy platform. ICMEg will organise workshops to reach European endorsement. The CUDS are a set of knowledge-based keywords and values with metadata that transcend scales and methods. It allows defining common language and terminology enabling seamless communications between different applications. The main issue here is the mapping of application specific settings and keywords to a standard and default set, namely the CUDS, so that an application agnostic approach to the development of multiscale science can be facilitated. Regardless of the specific applications integrated, the same set of API and CUDS keywords can be used. In this way, users may focus on the science instead of on the specific technical details of the applications. The CUDS enable the development of inter-process and inter-scale communications in a standard and open manner. The interfaces will be developed in compliance with the GNU LGPL license, or a more permissive license, to allow their interaction with open-source as well as with commercial packages. This will ensure sustainability over time through an open development process. In addition, three new and improved pre- and post-processing and scientific visualization tools will be further developed and integrated within the environment. These are AViz for publication-quality rendering of atomistic and electronic modelling data, Open nCAD-fluid for CAD-like pre-processing capabilities targeted at nano- and microfluidic applications and Mayavi2 for processing for complex visualization.

Integration of codes

In the first step, wrapping of computational tools will be designed based on indirect operations through file input and output (File-IO) without requiring any alteration to the native code of the respective integrated applications. The File-IO is not expected to be efficient for all production run scenarios due to its high IO overhead. It nevertheless offers an excellent platform for rapid development and debugging of new methodologies for concurrent modelling, and provides an efficient means for sequential multi-scale models, where moderate and infrequent data exchange is required. In the second step, the internal interfaces of the respective computational tools will be modified to allow the wrapper a direct access via a library interface to the internal state of the simulation tools. The internal interface library will allow the models to communicate through the defined common API and CUDS on a level that allows seamless integration and development of efficient inter-process and inter-model communications in particular for concurrent coupling of simulations.

Linking and coupling of models

One of the fundamental and challenging issues that will be tackled in SimPhoNy pertains to the question of consistency and reversibility between models applied to all scales, especially when the multi-scale modelling approach is connecting two methods having only a small subset of the degrees of freedom in common (e.g., atomistic and continuum). The work will therefore focus on investigating the loss of information, its impact on the accuracy, and how it may be remedied by enhanced coupling schemes. The SimPhoNy platform will provide a rapid development environment where intricate schemes for data reduction, extraction and transfer between models and methods can be easily and rapidly developed, and consequently tested and validated. Linking and coupling of models will cover problems requiring both direct transfer of properties from one model and computational method to another and more complex concurrent scenarios requiring extraction, averaging and filtering of data between two or more models. Simple examples include transfer of atomic positions from MD to DFT, or global rheological properties from one system to another. Besides model development and integration, SimPhoNy also includes elements of validation by comparing simulation data against a set of experimental test cases that will be performed within the project by manufacturing end user partners.

Project Acronym and Number: SIMPHONY 604005
Project Title: Simulation Framework for Multi-Scale Phenomena in Micro- And Nanosystems
Start and End Dates: 1.1.2014 -- 31.12.2016. EU Contribution: € 3,208,999.75
Coordinator: Dr. Adham Hashibon, Fraunhofer IWM, adham.hashibon@iwm.fraunhofer.de

Modelling in DEEPEN 604416

Subject of the modelling
Future nanoscale electronic and photonic devices

Physics/Chemistry Models used
Electronic: DFT plane wave and tight-binding (TB) models; Empirical TB model; DFT and empirical TB with Non-Equilibrium Green's Function (NEGF); k.p model; Drift-diffusion model;
Continuum: Electronic Device models

Simulation software and type of numerics used
VASP, OpenMX, Wannier90; TiMeS (DFT and NEGF), OMEN (TB); Tyndall TB and k.p models; TiberCAD (TIBER) drift diffusion models; S-Device (Synopsys) device modelling (TCAD)

Achievements of the model beyond experiments
Photonic and electronic device design requires detailed properties of nanoscale regions that are difficult and expensive to obtain experimentally. DEEPEN will develop a library for material properties and also develop models incorporating how these material properties change on nanometre length scales. To this end, models will be linked and coupled which have already proved very effective in describing phenomena at different levels of approximation and at different length scales. The linked models can be used to provide new insights as well as improved device design capability.

Application
Nanoscale electronic and photonic devices, in particular advanced CMOS and LED design

Relevant review articles

1. Mathieu Luisier, "*Atomistic simulation of transport phenomena in nanoelectronic devices*",
2. Chemical Society Reviews, Volume 43, Issue 13, pp. 4357-4367 (2014)
3. Matthias Auf der Maur, Alessandro Pecchia, Gabriele Penazzi, Fabio Sacconi, Aldo Di Carlo, *"Coupling atomistic and continuous media models for electronic device simulation"*, Journal of Computational Electronics, Volume 12, Issue 4, pp 553-562 (2013)
4. Matthias Auf der Maur, Gabriele Penazzi, Giuseppe Romano, Fabio Sacconi, Alessandro Pecchia, and Aldo Di Carlo, *"The Multiscale Paradigm in Electronic Device Simulation"*, IEEE Trans. Electron Devices, 58, n.5 (2011)

Summary of project

DEEPEN addresses problems common to future nanoscale electronic and photonic devices, providing an atomic-scale description of selected critical regions e.g. in the channel of a nanoscale transistor or active region of an LED while using continuum-level electronic models to describe the full device structure. DEEPEN also addresses the considerable uncertainty in many critical parameters required for device optimization.
DEEPEN will develop an open multi-scale modelling environment to simulate electronic transport processes in nanoelectronic and nanophotonic devices. The simulations will treat critical device regions using ab-initio calculation techniques, or, for larger critical regions, using empirical (tight-binding) methods. The interface between models is designed to be open and re-usable with a wide range of existing codes. An open source Common Data Format (CDF) is being defined and relevant metadata keywords will be defined in order to allow the exchange of data of different kinds (mesh associated or global quantities, physical and geometrical parameters). The environment will be demonstrated by integrating a range of open source and proprietary codes (electronic and continuum), which have the well-established capability to calculate phenomena at different levels of description. Although demonstrated with specific codes, it is envisaged that the interface should also be usable across a range of other codes with suitable adaptation of the code linkages to the interface.

Summary of Modelling

DEEPEN will implement linking and coupling schemes for a range of different models from ab-initio through to empirical tight binding and charge carrier diffusion codes.

Linking models

Several models will be linked (i.e. loosely coupled), with the output from the lower level being used to determine the input for higher level models. First principles electronic structure calculations will be used to determine details of carrier localisation. These empirical local electronic structure calculations will then be incorporated into a generic tight binding model applied to vertical transport and will also form the basis for a hopping model to describe lateral transport in InGaN quantum well structures. Linked simulations of TB code OMEN and continuum (device) SENTAURUS will use parameters extracted from more detailed studies performed on smaller structures, including ab-initio calculations.

Coupling models

In order to accurately describe selected nanoscale regions, model coupling will be implemented between first principles DFT codes and DFT code (TiMeS) and Tight-binding code OMEN applied to the transport. Both "transport codes" will be set up to accept Hamiltonian input in a tight-binding DFT format e.g. directly from OpenMX or from VASP, with the VASP plane-wave output converted to a localised basis using e.g. Wannier90. The output from the transport codes will then be fed back to the DFT codes to allow self-consistent calculation of the electronic structure and transport properties. Coupled simulations of OMEN and Sentaurus Device will be used when feedback effects from the macroscopic level to the nanoscale (e.g. by electrostatic interactions) are important in electronic devices, and fully self-consistent simulation of the system may be required. Coupling of models will also be required to investigate carrier tunnelling between neighbouring quantum wells in a multi-quantum well LED structure. The electronic tunnelling models will be implemented by developing TiMeS to treat tunnelling through the barrier between neighbouring quantum wells. To investigate the role of inter-well tunnelling in determining the steady-state carrier distribution in a MQW structure, this tunnelling model will be tightly coupled to TIBERLab's software, TIBERCAD as an example of an existing drift diffusion code.

Interfaces and Platform

TiberCAD as well as S-Device are closed-source commercial products. The general output format which we are developing should be adaptable for use with open source TCAD software, which could be used as a substitute. The interface developed in DEEPEN will be open source, allowing others to use existing commercial software or to adapt open source TCAD software for use with the DEEPEN platform. Together with 5 other NMP projects on multi-scale modelling (ICMEg, MMP, MODENA, NANOSIM and SIMPHONY) communication standards (metadata keywords and an overall data structure for file based information exchange) will be elaborated. These will be used in the DEEPEN platform. ICMEg will organise workshops to reach European endorsement. Once established, the platform will be widely applicable across a wide range of applications. The project's OS environment will be released under the GNU Lesser General Public License (GNU LGPL), ensuring that the core of the multiscale environment together with all its Application Programming Interfaces (APIs) can be distributed and even modified freely. It will also be available through TIBERLab's existing support environment www.tibercad.org.

Project Acronym and Number: DEEPEN
Project Title: From atom-to-Device Explicit simulation Environment for Photonics and Electronics Nanostructures
Start and End dates: EU contributions:
Coordinator: Eoin O'Reilly, Tyndall National Institute, eoin.oreilly@tyndall.ie

Modelling in MMP 604279

Subject of the modelling
Materials processing of copper-indium-gallium-selenide type thin film photovoltaic (PV) cells and of phosphor converted lighting systems (phosphor LEDs)

Physics/Chemistry models used

Electronic:	None
Atomistic:	None
Mesoscopic:	None
Continuum:	Fluid Dynamics (CFD), Continuum mechanics and thermal models, Computational thermodynamics, Phase field models, Optical models (scattering, ray-tracing)

Simulation software and type of numerics used

Continuum:	X-stream: Multi-physics CFD (finite volume), Comsol multiphysics (finite element), MICRESS: phase field software (finite differences), Optical modelling software: VTT in-house scattering code, HOMAT (finite element)
Database:	CALPHAD thermodynamics database and interpolation software, Thermo-Calc software package for thermodynamic calculations

Achievements of the model beyond experiments
The development and design of materials and systems for solid state lighting (SSL) and photovoltaics (PV) requires a structured product design methodology. Such multi-objective and multi-disciplinary optimization can only be realistically achieved by a combination of dedicated numerical approaches addressing proper physics at the proper length scales combined with some experimental input.

Application
Solid state lighting and photovoltaic applications in diverse fields, including ambient lighting, healthcare, textile integration and PV power plants.

Relevant review articles

1. Schmitz, G. J.,Prahl,U., ed. (2012). Integrative Computational Materials Engineering- Concepts and applications of a modular simulation platform. Wiley VCH Verlag. ISBN 978-3-527-33081-2.
2. J.R. Stewart, H.C. Edwards: A framework approach for developing parallel adaptive multiphysics applications, Finite Elem Anal Des, 40 (12) (2004), pp. 1599–1617
3. S.G. Parker, D.M. Beazley, C.R. Johnson: Computational steering software systems and strategies, IEEE Comput Sci Eng, 4 (4) (1997), pp. 50–59
4. J. R. Frisvad et al., Computing the scattering properties of participating media using Lorenz-Mie theory, ACM Transactions on Graphics, Vol. 26, Issue 3, Article No. 60, 2007
5. Hong Du, Mie-scattering calculation, Applied Optics, Vol. 43, No. 9, 1951-1956, 2004

Summary of project
MMP develops an open source platform for linking of continuum materials models applied to different scales and including multiphysics phenomena. The MMP platform interfaces to the computational tools and their libraries and to data repositories through dedicated modules. The platform design is generic, even though its use will be demonstrated on case studies involving only continuum based models. Its design allows to link and couple different models. The object-oriented design of platform uses metadata representations of properties, fields and functions, naturally hiding internal representation behind a common interface.

The strategy is to equip existing software and databases with general application interfaces (APIs). These APIs ensure compatibility with the MMP-platform and allow for data exchange and control. The API definition will be open, thus any software provider can build an API for their solution to achieve compatibility with the MMP platform. The general application interface of the MMP-platform will be based on the Multi-Physics Integration Framework (MuPIF); a prototype, open source integration platform.

In order to achieve a sustainable and flexible platform design, standardisation of metadata keywords and data structures is essential. Collaboration with other funded projects should ensure agreement on these keyword and standard interface definitions.

The MMP platform will enable the user to automatically execute simulation scenarios, i. e. problem specific process flows of the desired multiscale-multiphysics simulation. It sequences the required simulation services and specifies the timing of the individual simulation processes. This is especially important for parallel computing, and for iterative schemes required for convergence and optimization. Code linking is handled through dedicated algorithms embedded in the MMP-platform. These operations can be called in the simulation scenario.

Two case studies will be considered: the materials processing for photovoltaic cells and phosphor converted LEDs. These applications require linking of codes for the microstructure (phase-field methods) to continuum models for the macro and device scale. < you link codes, not results; microstructure is the result of a phase field model) Also the project involves multi-physics coupling of thermal and optical modelling.

Homogenisation and scale transitions

An embedded toolbox will be developed and implemented which enables the required scale transition relations, e.g. spatial mapping, interpolation and homogenization algorithms that transform spatially resolved information provided by models at lower scales of resolution to properties for models at upper resolution levels.

The homogenization and scale transition techniques will be integrated in the platform as additional applications. Such an abstract concept retains the plug-and-play design, allowing the combination of different simulation tools, scale transition algorithms, etc. In this sense the scale transitions are independent of the (numerical) solution technique (e.g. FEM, phase field, molecular dynamics, etc.) used to resolve one scale. The homogenization facilitates the calculation of an effective property based on a field in a finite volume, where interpolation generates a continuous field based on values defined in a finite number of points only. The sequencing of the analysis of the different scales is flexible in the platform, e.g. a fully nested solution can be obtained where the two scales are solved simultaneously, but also a consecutive approach where for example first the large scale and then the fine scale is resolved.

In order to achieve a sustainable and flexible platform design, standardisation of metadata keywords and data structures is essential. Collaboration with other funded projects should ensure agreement on these standard interface definitions.

In order to promote and diversify plug-in possibilities, the MMP platform will be distributed under an Open Source public license (for instance, GNU Lesser GNU Public License (LGPL)) that allows a broad distribution of MMP but protects the intellectual property encoded in the APIs (or glue codes) and service modules. The license should also facilitate the interfacing with commercial (or non-public) software, without disclosing the source code or intellectual property of this software, even in case a direct interfacing based on direct access to data fields and libraries is required.

Project Acronym and Number: MMP 604279
Project Title: Multiscale Modelling Platform: Smart design of nano-enabled products in green technologies
Start and End Dates: 1-1-2014 to 31-12-2016. EU Contribution: 3,339,235 €
Coordinator: Dr. Jan-Paul Krugers, TNO, jan-paul.krugers@tno.nl

Modelling in NANOSIM 604656

Subject of the modelling

Nano-structured reactive porous particles; virtual prototyping of a complete value chain from particle design to the associated large scale reactor systems

Physics/Chemistry models used

Electronic: DFT to simulate reactions of oxygen and/or hydrocarbons with various metals or metal oxides; reaction enthalpy and activation energies of fundamental single-step processes at the atomistic scale that occur at approximately picosecond timescales in order to parameterize KMC or continuum reaction models.

Atomistic: Classical molecular dynamics (MD) to simulate diffusion processes (e.g., through metal oxide layers). Kinetic Monte Carlo (KMC) to simulate reactions and complicated multistep processes that occur at approximately microsecond timescales, such that final reaction mechanisms and parameters for continuum reaction can be derived.

Continuum: CFD 1 level: CFD coupled with particle dynamics (DEM) and intra-particle continuum models to simulate temperature and concentration profiles within and around porous particles. This allows the development of drag, heat, and effective reaction rate models, taking key phenomena (e.g., particle clustering) into account. CFD 2 level: Multiphase Euler-Euler CFD to simulate particle clustering CFD 3 level: Multiphase Euler-Euler CFD to simulate full-scale equipment

Process model: Phenomenological models to simulate full-scale equipment and systems

Simulation software and type of numerics used

Electronic: VASP (Plane-wave DFT)

Atomistic: SPPARKS (KMC), LAMMPS (MD)

Continuum: Classical finite-volume CFD sw: NEPTUNE_CFD, ANSYS FLUENT, OpenFOAM, Particle

Dynamics sw: LIGGGHTS (DEM) and CFDEMcoupling (DEM+CFD), Finite-difference sw for reactive intra-particle diffusion & heat conduction: ParScale

Finite-difference sw: for full-scale conservation equations: PHENOM

Achievements of the model beyond experiments

With the help of tools developed in NanoSim, process optimization or intensification tasks can be performed computationally with high confidence and with less effort. Filtered fluidized bed reactor and phenomenological process models capable of economically simulating industrial scale units with a high degree of accuracy and generality will allow fast and efficient virtual prototyping of new process concepts at full industrial scales and significantly accelerate the traditional scale-up and demonstration process of promising new reactor concepts.

The simulation-based nano-structured material design will enable selection of highly reactive, mechanically stable, and sinter-resistant materials reducing lengthy and costly experimentation.

The NanoSim's co-simulation tool (i) offers a single open-source co-simulation environment for gas-particle multi-physics simulation, (ii) is user friendly, flexible and hence can be quickly adapted to new applications, and (iii) its parallel implementation will allow researchers to attack extremely demanding simulations which are currently too time consuming, or simply inaccessible due to memory limitations. Data generated by NanoSim's tools (e.g., for phenomena happening at a single particle scale) can be analysed on the fly, and collected in a format that can be used directly as an input in the next level of modelling.

Application

Chemical Looping Reforming (CLR) for hydrogen production with integrated CO_2 capture. Moreover, the NanoSim methodology can be applied to any (reactive) gas-particle contacting processes involving heat & mass transfer (catalytic or non-catalytic). Examples for such processes would be biomass reactors, drying processes, coating processes, as well as other processes in the food/pharmaceutical/chemical/energy industries.

Relevant review articles covering the topic

1. Adanez, J., et al., Progress in Chemical-Looping Combustion and Reforming technologies. Progress in Energy and Combustion Science, 2012. 38(2): p. 215-282.
2. Norskov, J.K., et al., Density functional theory in surface chemistry and catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2011. 108(3): p. 937-943.
3. Sundaresan, S., Modeling the hydrodynamics of multiphase flow reactors: Current status and challenges. AIChE Journal, 2000. 46(6): p. 1102-1105.
4. Van der Hoef, M., et al., Numerical simulation of dense gas-solid fluidized beds: a multiscale modeling strategy. Annual Review of Fluid Mechanics, 2008(40): p. 47-70.

Summary of project

A key objective of the NanoSim project is to create an efficient and cost effective multi-scale simulation platform which incorporates of a set of interconnected free and open-source codes. To support the information flow and data sharing between different simulation packages, the NanoSim project will develop an open and integrated framework for numerical design (i.e., a common software environment) called Porto. Specifically, Porto is the key software tool which handles data and associated meta-data, and has an application programming interface (API) to ensure extensibility. This software will be used and distributed in terms of the GNU Lesser General Public License (LGPL).

The NanoSim project develops coupling (concurrent modelling) for which a co-simulation platform (COSI) is developed as well as linking (sequential modelling) methods. In the linking scheme information will be exchanged offline between different continuum models via newly developed constitutive equations. The different formats and interfaces used in the NanoSim project will conform to industrial standards (e.g., ECMA-404's JSON format) to enable the future implementation in a larger and extendable framework architecture.

A data centric strategy for linking and coupling of models is adopted. In Porto, a database of meta-data is built that describe the models and their applications in terms of entities and relationships supporting (correctly, safely and maintainable) sharing data between multiple in-house and commercial tools (proprietary and open). The strength of this framework lies in the code management and maintenance as requirements change and the platform grows with new tools and methods.

A new homogenisation tool called REMARC will be used in the linking between 1) electronic and atomistic models (DFT and KMC and MD), as well as 2) between atomistic and continuum models. The newly developed tool *CPPPO*, for homogenisation of Computational Fluid Dynamics (CFD) data, will link continuum models applied to different scales. The novelty is that the workflow for homogenisation using these tools will be largely automated through the use of *Porto*. To link the continuum models, constitutive equations will be developed based on small-scale simulations results, and will be validated with experimental results. Semi-automated reversibility checks will be performed to guarantee model consistency. The approach will allow one to compare the "fine scale" and "coarse scale" simulation results and tune the model if necessary. The novelty of Porto is that the tool will offer an automated workflow for the generation of new closures (constitutive equations) for continuum models. Model coupling (or concurrent modelling) in NanoSim involves the coupling of particle dynamics models (i.e., using the Discrete Element Method, DEM), classical Computational Fluid Dynamics (CFD) flow models, and intra-particle continuum models to predict reaction-diffusion processes within a porous particle. Specifically, the Co-Simulation (COSI) platform will enable coupled simulations of reactive gas-particle flows, in which relevant intra-particle data (e.g., the reaction rate within a particle) is passed to the CFD flow model during a single simulation run. In addition, intra-particle processes may change particle properties (e.g., the size and density of a particle). COSI will also be able to hand over such data to the particle dynamics model, and hence enable fully coupled gas-particle simulations.

Project Acronym and Number: NanoSim (604656)
Project Title: A Multiscale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials (NanoSim)
Start and End Dates: 01/01/2014 – 31/12/2017. EU Contribution: €3,888,000.00
Coordinator: Shahriar Amini, SINTEF Materials and Chemistry, shahriar.amini@sintef.no

Networking in ICMEg 606711

Subject of the project
Standardization of data exchange between models and respective simulation tools in Integrated Computational Materials Engineering settings

Physics/Chemistry models being considered

Electronic:	DFT
Atomistic:	MD
Mesoscopic:	discrete Phase Field, discrete models for thermodynamics and dislocation dynamics
Continuum:	continuum Phase Field models, models for thermodynamics, thermo-mechanics, fluid-flow, crystal-plasticity model, …

Empirical models generated
Simulation chains will be able to calibrate existing or to generate new constitutive equations.

Simulation software
A thematically structured directory of available simulation software tools will be compiled.

Achievements of the model beyond experiments
Virtual description of entire evolution of microstructures, properties of materials, properties of components, prediction of life-cycle behaviour

Application
Materials development, process development, alloy design,

Relevant review articles covering the topic:

1. National Research Council: Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security; National Academic Press, Washington, D. C. (2008), ISBN: 0-309-12000-4.
2. G.J. Schmitz and U.Prahl (eds): Integrative Computational Materials Engineering- Concepts and applications of a modular simulation platform, Wiley VCH Verlag Weinheim, ISBN 978-3-527-33081-2 (2012)
3. TMS: Implementing ICME in the Aerospace, Automotive, and Maritime Industries (2013) Downloadable for free from: http://www.tms.org/icmestudy/

Summary of the project
ICMEg as a CSA is a networking project aiming to build and maintain a network of stakeholders in Integrated Computational Materials Engineering (ICME) and to define an ICME language in form of an open and standardized communication protocol. This can be used by third parties to create a “plug & play” type architecture which will

- Significantly facilitate the exchange of data between different tools
- Create new options and functionalities of the present tools
- Allow for easy integration between commercial and academic approaches
- Provide the pathway for life-cycle modelling of components/products
- Allow for global optimisation of process chains
- Stimulate many further new developments

Summary of the materials model communication standard activities
The project focusses on models to describe microstructure evolution as a central part of ICME. Microstructure properties depend on the entire process history as well as on shape of the component and on the actual alloy composition. Outlining a scale and process spanning modelling scenario and making it available for material-by-design is one of the key objectives of ICME.

This networking project will have workshops to reach European endorsement for communication standards being proposed and jointly elaborated within 5 other NMP projects on multi-scale modelling: DEEPEN, MMP, MODENA, NANOSIM and SIMPHONY.
These standards will include a generic and structured list of metadata keywords and an overall data structure for file based information exchange. These will be based on existing standards to the largest possible extend and will allow sequential i.e. file based interoperability. ICMEg will propose Communication Standards for a file based exchange of information between models describing the behaviour of

- the components providing the boundary conditions for the evolution of the microstructure
- the microstructure comprising multiple grains and multiple phases
- the individual phases and their properties

The standards and interoperability scenarios developed in ICMEg will focus on coupling and linking 2D and 3D continuum models but data obtained from e.g. DFT, MD and other small scale models will be integrated into the scenario. ICMEg will also elaborate standards for inclusion of data from electronic/atomistic/mesoscopic models required for continuum model simulations. Discrete models will be linked to give effective values to continuum models. Discrete models could e.g. deliver thermodynamic data for the individual phases in complex alloy systems, data for thermal conductivities or anisotropic thermo-mechanical properties and also provide relevant data like critical nucleation undercoolings for the formation of phases. Homogenisation tools with interpolation schemes to calculate effective properties from model output can be included in the scenarios.

Based on the identified needs of the continuum models, missing functionalities will be identified and a roadmap for future developments in the area of discrete and continuum models will be proposed.

The communication standards to be developed will be extendable and also applicable to other applications. They will provide the basis for a future platform which will enable simultaneous (coupling) or consecutive (linking) execution of models. The actual development of platforms is however not part of ICMEg but takes place within the EU projects mentioned above and hopefully the standards and platforms will be adopted by a wide community in the future.

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