MMP

PROJECT FINAL REPORT

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1   Final publishable summary report

1.1   Executive summary

The MuPIF platform

The MMP (Multi-scale Modelling Platform consortium has developed an integrating modelling platform, especially equipped to target multi-scale and multi-physics scientific and engineering problems, the MuPIF platform. The innovation of MuPIF lies in its generic and modular character, supported by data standardization and proper definition of application interfaces. This allows for the integration of new and existing modelling software's and data repositories as plug-in components. MuPIF has been distributed as open source software supported by online documentation. This enables future users, e.g. SMEs, to join, contribute and benefit from the MMP-project.

The MuPIF platform provides the European industry with a competitive advantage by allowing for an integrated process, material and product design. Multi-scale modelling and design will considerably reduce development costs, decrease time to market and improve process yield and device functionality. Moreover, the cloud computing strategy enables the optimal utilization of simulation facilities and facilitates collaboration.

The MuPIF platform has been developed and improved throughout the project to meet TRL5 status, achieved in October 2016. A website has been launched for public use on http://www.mupif.org.

Showcases

Case 1 "LED" is to develop a multiscale modelling scheme that will help to optimize the design of phosphors as light conversion material and to compute the light output, taking heat dissipation into account. The main parameters varied were the green and red phosphor concentrations in the silicone mixtures. The results obtained showed that the trend in the response is well reproduced by the developed model, but some calibration is required to acquire good correspondence with the experimental measurements. The platform's design is open and generic making possible to tune new scenarios (e.g. LED package geometries, optimization routines, simulation chains, etc.) with ease in order to adapt to changing market needs.

Case 2 "CIGS" is to perform multiscale simulations of the selenization process for CIGS thin film production at the process/component scale and at the scale of the material microstructure. The script performs a direct linking of the macro simulation X-stream (CelSian) and the micro simulation MICRESS (Access). The demonstration is based on a prototypic simulation run comprising a macroscopic furnace simulation (X-stream), 25 microstructure simulations on different characteristic locations on the precursor film (MICRESS), data exchange between the different simulation tools via the platform and different platform related services as the quality factor evaluation and homogenisation schemes for data interpolation.

The MuPIF platform can of course be used for many other applications. Outside the context of the MMP project, the MuPIF platform has already been used for the following cases: Polymer-matrix composite materials, Effect of fire on structural response, Moisture condensation in tunnels Strain effects on quantum transport using multiscale modeling.

1.2   Project context and objectives

Multiscale methods have contributed to a considerable progress in bridging the field of mechanics of materials to the field of materials science. In this case it is mainly due to a fruitful combination of micromechanics and mathematical approaches, with a steadily increasing multi-disciplinary character. Recent developments in nanotechnology are rapidly changing synthesis and manufacturing processes, e.g. directed molecular evolution or self-assembly. This fuels the need to extend the envelope of modelling at multiple scales to allow for material, process and device design through a scale-integrated approach.

The dissemination of these newly developed simulation capacity to the industry however, is at a slower pace. Several technical and scientific challenges can be identified, see Table 1. The scientific challenges are complex multi-physical interactions, which require a solid understanding on description of the physical phenomena, and most importantly, describing the effects of underlying nano- and micro-mechanisms on the system behaviour.

Table 1: The challenges in utilizing advanced computational techniques.

Scientific challenges	Technical and practical challenges
Description of physical phenomena addressed at the proper length scales, from nm to the system level. Different models are needed to handle all.	Multiscale models currently have hardware dependent, problem specific implementations.
Coupling of nano scale effects to the macro world. Proper formulations are needed to handle scale separations.	Combining different software packages, I/O management in different programming languages.
Multi-physical relationships operating at different length scales.	Standards on data interfacing and storage are lacking, which results in undesirable patching, data losses and re-works.
Error estimation for homogenization techniques and non-linear problems.	Expertise on process and modelling software is geographically distributed.
Evolution of architectural framework in combination with the evolution of plug-in components.	Too slow transfer of modelling methods developed by academia to industry, to answer changing industrial needs.

On the technical side there is an evident lack of standard tools and methods for multiscale modelling; such that for every different scheme, a different implementation is needed. Additionally, fully nested homogenization schemes often provide best accuracy at the expense of computational efficiency. New approaches, such as reduced order modelling, are needed to trade off industrial operation level accuracy to the available computational capacity.

Hence there is a strong need for an open environment that can combine different computational tools and can handle the scale differences in a computationally efficient and accurate way.

MMP-objectives

The MMP-project aimed at answering these needs by developing an open source platform to utilise multiscale modelling. The platform should enable integration of different software packages designed to model specific physical phenomena individually to comprehensively simulate a nano-enabled product. The general platform concept is shown in Figure 1. The key properties of the platform are listed in the blue box. The main user properties of the user interface module are highlighted in the orange box.
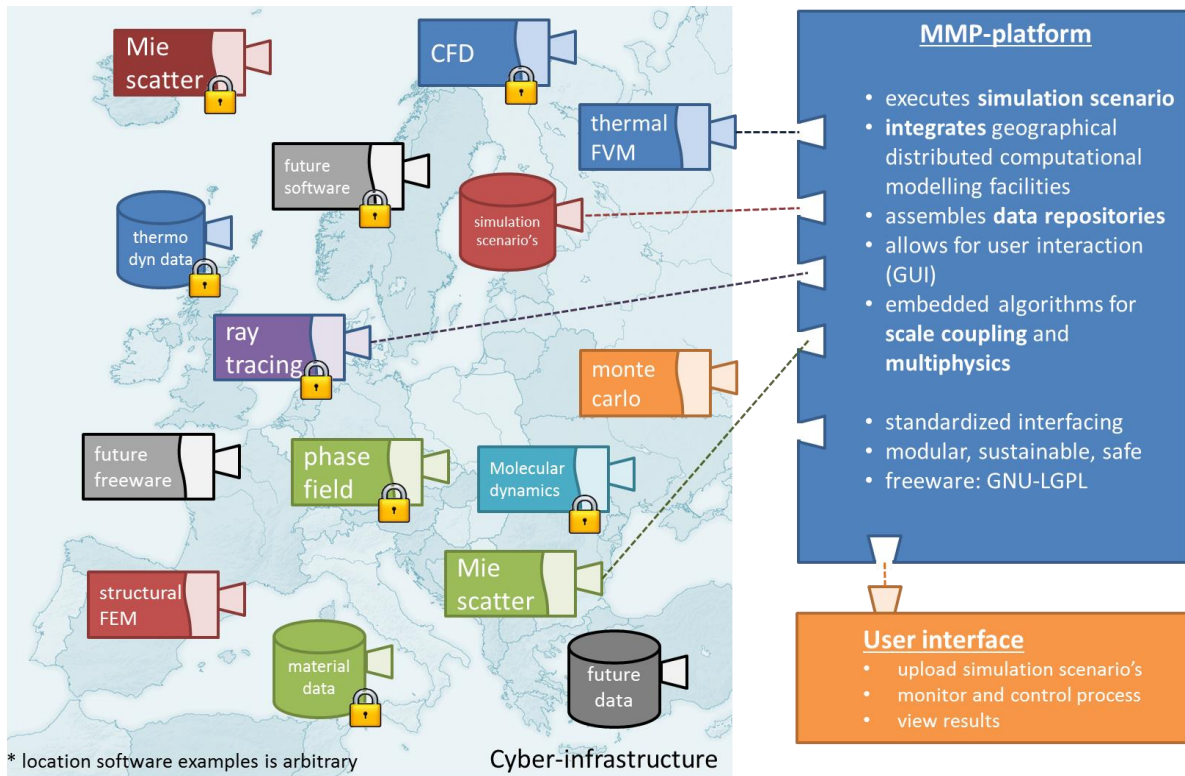

Figure 1: Schematic representation and vision of the multiscale modelling platform. Individual software solutions (open and/or commercial, indicated by the lock-symbol) will be extended by an open and standardised application interface API (indicated by the handles on the right side of the icons) which allows distributed communication with the MMP.

The MMP project integrates the computational facilities, which are in general geographically distributed. Computational facilities entail modelling software, licenses, computer hardware, data repositories but also the very essential expertise. The strategy is to make computational services available, by equipping existing software and databases with a general application interfaces (APIs). These APIs (or glue codes) ensure compatibility with the MuPIF-platform used in MMP project to steer individual applications and enable mutual distributed data exchange. The API definition will be open, thus any software provider can build an API for their solution to achieve compatibility with the MuPIF platform.

The general application interface of the MMP-platform has been based on Multi-Physics Integration Framework (MuPIF); a prototype, open source integration platform developed at Czech Technical University in Prague (CTU).

In order to achieve a sustainable and flexible platform design, standardisation of data flow format is essential. The standardisation is required within the MMP project, but it also should be consistent and compatible with standards being developed in the broader modelling community.

The target results of the platform development are:

- To develop an integration platform, allowing combining individual simulation tools into a complex, multi-physics simulation.
- To design a generic Application Interface allowing abstract data exchange and steering of individual applications.

Use cases

Industrial innovation is focusing on clean energy alternatives, products with lower carbon footprint and lower energy consumption. The efforts concentrate both on improving process technologies as well as improving product efficiency, increased life-time and reliability. Multiscale systems engineering will play an essential role in achieving these goals, since it has the premise to reduce development times/time-to-market, reducing trial-and-error runs, increase product performance, increase production yield by optimizing process conditions.

The MMP-platform aimed for, needs to be employed for a wide range of multi-scale engineering problems. This flexibility provides the opportunity to assess case studies which focus on one of society's pressing issues of our time, energy. Alternative energy sources with low carbon footprint or more efficient ways of energy use are essential for a sustainable society. Nano-enabled materials and devices can be brought to bear on the latter problems, to develop clean energy generation and energy efficient devices. Motivated by this energy-challenge, two case studies on nano-enabled products with a high environmental impact have been addresses for the validation of the platform:

    i.   copper-indium-gallium-selenide (CIGS) type thin film photovoltaic (PV) cells, and
   ii.   phosphor converted lighting systems (phosphor LEDs).

Figure 2: The bright future of nano-enabled devices: thin film CIGS solar cell (left) and design freedom of high power LEDs (right).

Both products combine different type of physics, i.e. thermal, mechanical, chemical, optical etc., operating at length scales varying from molecular level to a system level. Using MMP, a better understanding on the underlying mechanisms across different length scales of the product and process are provided. This enables multi-level decision making and thereby, adequate product and process optimization. By choosing disjunct multiscale simulation scenarios the general benefit and

applicability of the MMP for multiscale and multi-physics simulation challenges posed by nano-enabled products can be shown and underpin the future dissemination of MMP into further areas of application.

These case studies will demonstrate the ability of the MMP-platform to unify the knowledge, initially scattered over independent institutes and companies, into one integral design platform. Small and medium size enterprises (SMEs) can also join and contribute due to the relatively limited effort and resources required, to connect initially independent (mature) modelling software.

MMP has the following scientific and technological objectives:

(1) Integrated multi-scale modelling platform
- Developing an open-source platform for the integration of software systems / modules to a joint multiscale modelling framework, which will be an integration tool, allowing combination of different modules to build tailor-made multiscale and multi-physics simulations.
- An accurate mathematical description of scale transitions for relevant physical parameters. Implementation of homogenization schemes and multi-physics relationships, such that each module handles different length scales, and passes relevant variables to other modules.
- Active control on computational efficiency using reduced order modelling.

(2) Software engineering, platform implementation
- Developing a generic General Application Interface, which will manage individual modules.
- Collaboration with other funded projects to make standard interface definitions. High-level description of plug-in component interfaces, as defined by these standards.
- Transparent distributed developed software and documentation through Wiki based MMP-project page.

(3) Phosphor converted lighting systems
- Developing an opto-thermal multiscale modelling scheme for design optimization of LED devices using phosphors as light conversion material, which computes the system level light output, taking heat dissipation into account.
- LED-system optimization with respect to the phosphor light conversion system, e.g. position in the device, composition of the phosphor encapsulant composite, phosphor blend, etc.
- Experiments to validate simulated spatial distribution of optical intensity and thermal fields.

(4) CIGS processing
- Developing a multiscale process simulation for thin film CIGS selenization, ranging from atomistic Se-diffusion, nm-scale interface motion during crystallisation and phase formation in CIGS up to furnace level simulations and device level efficiency.
- Improved material deposition and process conditions for large area deposition of high quality CIGS layers, yielding increased device efficiency, increased production stability, reduced material and energy use in production.
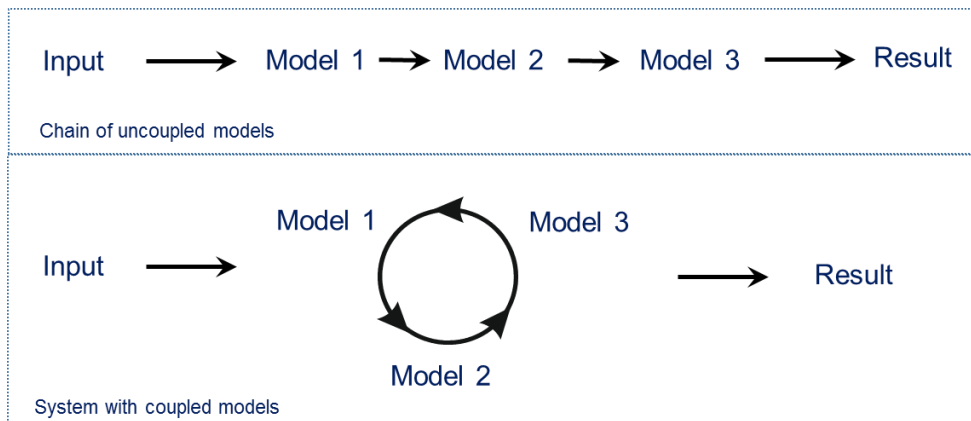- Validation of the integrated model on device level and sub-process level.

1.3　Main scientific and technology results

1.3.1　Introduction

Many (multiscale) problems are strongly coupled of which the interdependence is essential, and there is a need to achieve a global convergence in every step, before going to next one, which is not

achievable by simple chain. So the main advantage of 'on-the-fly' multiscale modelling instead of an uncoupled chain of single scale models for device optimization are (depending on application) is that one can simulate the real process instead of just taking into account a linear influence. In many production processes different physical changes occur at different points in time at different scales, but they are influencing each other. This means that the output of one model is the input for the second model, but also vice versa. In more complicated cases one could even think of three models that are coupled in this way. To do this manually by use of single models is a tedious, very complicated, time consuming task.

Input ⟶ Model 1 ⟶ Model 2 ⟶ Model 3 ⟶ Result

Chain of uncoupled models

Input ⟶   Model 1   Model 3   Model 2   ⟶ Result

System with coupled models

Showcases

Case 1 **"LED"** is to develop a multiscale modelling scheme that will help to optimize the design of phosphors as light conversion material and to compute the light output, taking heat dissipation into account. The main parameters varied were the green and red phosphor concentrations in the silicone mixtures. The results obtained showed that the trend in the response is well reproduced by the developed model, but some calibration is required to acquire good correspondence with the experimental measurements. The platform's design is open and generic making possible to tune new scenarios (e.g. LED package geometries, optimization routines, simulation chains, etc.) with ease in order to adapt to changing market needs.

The recently started ECSEL-project Delphi4LED, led by Philips, develops an electric datasheet for LEDs. The project team is interested in the MMP approach on how to take into account the heat produced in LED phosphor.

Case 2 **"CIGS"** is to perform multiscale simulations of the selenization process for CIGS thin film production at the process/component scale and at the scale of the material microstructure. The script performs a direct linking of the macro simulation X-stream (CelSian) and the micro simulation MICRESS (Access). The demonstration is based on a prototypic simulation run comprising a macroscopic furnace simulation (X-stream), 25 microstructure simulations on different characteristic locations on the precursor film (MICRESS), data exchange between the different simulation tools via the platform and different platform related services as the quality factor evaluation and homogenisation schemes for data interpolation. Simulation runs are completely orchestrated and steered by the MuPIF platform. Thermal CVD simulations can show a strongly coupled multiscale behaviour if the thermal process changes material properties (defined on a much smaller scale) in a way that it has an impact on the macroscopic solution. In particular, this would be true for the RTP selenization with predominant radiative heat transfer. In this case, the emissivity of the selenized sample effects the temperatures in

the furnace, the emissivity itself is determined by the phase transformations taking place on a microscopic scale. The same argument holds for the Se consumption in a conventional tube furnace selenisation process. The Se concentration in the gas ambient on the macroscopic length scale depends on the Se consumption controlled by phase transformation on a micrometer scale.

The MuPIF platform can of course be used for many other applications. Outside the context of the MMP project, the MuPIF platform has already been used for the following cases:

Polymer-matrix composite materials
MuPIF used as modeling platform in H2020 Composelector project focusing on development, demonstration and assessment of an integrated software platform based on a multi-disciplinary, multi-model and multi-field approach for decision-making in the selection, design and fabrication of micro-structured and macro-structured polymer-matrix composite materials.

Effect of fire on structural response
Platform is used to simulate the effect of fire on structural response, project GACR 16-18448S, where MuPIF serves as interoperability platform for simulation model consisting of CFD fire simulation and nonlinear solid mechanics simulation.

Moisture condensation in tunnels
Platform has been used to model moisture condensation in tunnels, project CESTI.

Strain effects on quantum transport using multiscale modeling
Quantum transport across nanostructures is of great importance for designing upcoming quantum technologies. When engineering new concepts there is a need to predict how deformation resulting from stressing of cooling devices might affect electronic transport. Currently we are exploring the link between molecular dynamics calculations for predicting strain to simulate those changes in transport using tight-binding numerical methods. In such approach the MuPIF platform is used to connect the LAMMPS and Kwant codes, for molecular dynamics and quantum transport simulations respectively.

1.3.2   Multiscale modelling platform development

The MMP projects uses MuPIF integration platform to steer the individual simulation tools and enable data format neutral data exchange in distributed environments. The platform is by design generally applicable to any multi-physics and multi-scale simulation workflow. The approach followed in the MuPIF platform is based on a system of distributed, interacting objects designed to solve given problem. The individual objects represent entities in the problem domain, including individual simulation packages, but also the high-level, complex data, such as spatial fields or microstructures. The abstract classes are introduced for all relevant entities in the model space. They define a common interface, called API that needs to be implemented by any derived class, representing particular implementation of specific component. Such interface concept allows using any derived class on a very abstract level, using common services defined by abstract class, without being concerned with the implementation details of an individual software component. The APIs have been defined for simulation tools and high-level, complex simulation data sets. This essentially allows to manipulate all simulation tools and complex data sets using the same interface. Moreover, as the simulation data are represented by objects as well, the platform is independent on particular data format(s), as the

exchanged data (such as fields and properties) can be manipulated using the same abstract interface. Therefore, the focus on services is provided by objects (object interfaces) and not on underlying data itself. The workflow developed in MuPIF-platform is defined by top-level script in Python language (called scenario) using the services provided by newly introduced classes. A graphical tool for workflow development and execution has been developed.

Even though the platform can be used locally on a single computer, the real strength of the MuPIF platform is its distributed design, allowing to execute simulation scenarios involving remote applications and data sources. The concept of so called proxy object that represent remote objects allows to hide all the details of remote data exchange and execution to the user. The communication layer is built on Pyro library, which provides a transparent distributed object system fully integrated into Python. It takes care of the network communication between the objects when they are distributed over different machines on the network. One just calls a method on a remote object as if it were a local object – the use of remote objects is (almost) transparent. This is achieved by the introduction of so-called proxies. A proxy is a special kind of object that acts as if it were the actual object. Proxies forward the calls to the remote objects, and pass the results back to the calling code. In this way, there is no difference between simulation workflow for local or distributed case, except for the initialization, where, instead of creating local object, one has to connect to the remote object. See figure 3 for an illustration.

The initial phases focused on identification of requirements, collected from the partners. These data consist of workflow descriptions, identification of needed models, data dependencies between models, steering services, and additional required platform services regarding licensing, user authorization, and security. The templated documents to describe envisioned workflows has been developed as well as questionnaires to collect the inventory of available simulation tools and their requirements. Based on the collected data from project partners, the initial API versions have been proposed and internally reviewed to ensure that all the requirements have been addressed.
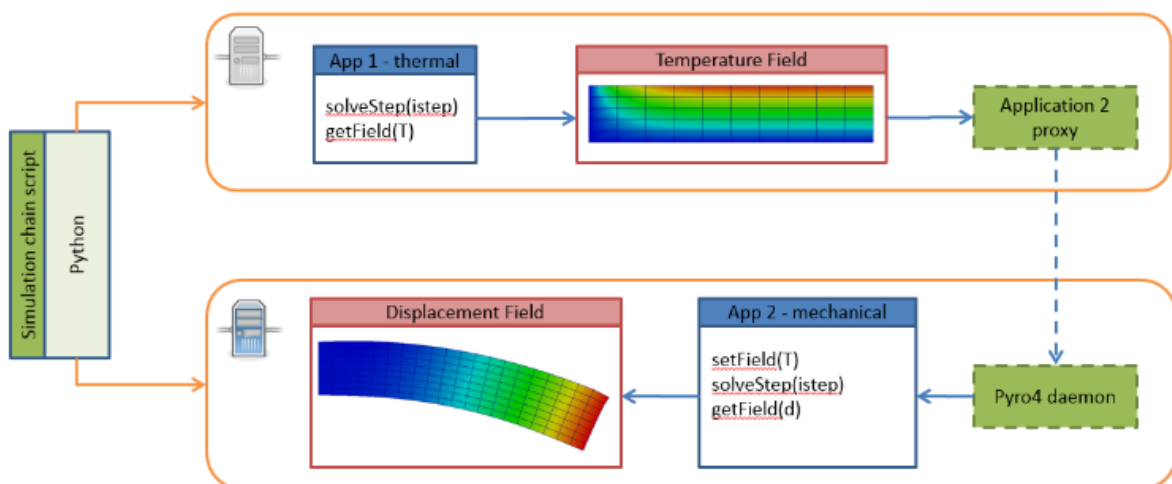

Figure 3: Example of distributed Thermo-mechanical workflow

Based on final API specifications, the further development of the platform started to provide missing functionality. The development of MuPIF platform, released under LGPL license, has been hosted on Sourceforge repository, providing software repository, user forum and bug tracking systems, which facilitated the platform development and interaction with users. The representations for unstructured grids and spatial (continuous) fields have been adapted to the extended requirements, additional types of interpolation cells have been implemented, as well as additional classes facilitating to develop complex workflows, such as solution steps, general functions, properties, or class representing units. VTK and Ensight IO filters have been developed.

To enable integration of different types of applications (in house, commercial, etc.) two different approaches have been developed and illustrated using examples. Direct implementation requires a simulation tool written in Python, or a tool with Python interface. In this case the required application interface will be implemented directly using direct calls to suitable application's functions and procedures, including necessary internal data conversions. The second option, called indirect approach, is based on wrapper class implementing application interface, using, for example, simulation tool scripting or I/O capabilities, allowing to connect standalone, closed source application, which is executed by the wrapper in each solution step.

To support distributed simulation workflows, the job manager has been implemented serving the allocation, steering, and monitoring of individual simulation tools. The SSH tunnelling approach has been developed and tested providing the necessary user authorization, data security, and optional tunnelling to bypass the strict networking policies. Later in the project, the support for Virtual Private Network has been added as well.

The platform has been successfully tested on distributed grid infrastructure, set up using the tools provided by the platform but also using the HTCondor middleware. The graphical tool has been developed to facilitate the definition of HTCondor workflow, their submission and monitoring.

Significant effort has been spent on maintenance of the platform itself. The user support has been provided not only to the project partners, to develop, test, and run case-studies build on the platform infrastructure. The platform documentation has been developed, consisting of User and Reference manuals. A set of automated unit tests has been developed to test functionality of all framework classes and their methods and compare them to the expected results to ensure the stability of platform releases. In addition, a number of demonstration examples illustrating the platform use have been developed as well to illustrate the platform use and serve as starting point for the new users.

Later in the project, the prototypic graphical interface for Condor job submission has been further extended in this period to allow graphical workflow modelling and execution monitoring, build on top of Eclipse framework. It allows the user to efficiently develop the workflow from provided common building blocks. The tool allows to include user defined code blocks for further customization and introduce user defined variables that can be modified interactively during the workflow execution. The GUI will be released as open source software.

Within the case studies specific scenarios have been developed, tested, and executed. The WP2 test case scenario consists of both optical and thermal models that simulate phosphor converted lighting systems (see also section 3.2). The optical model consists of Mie scattering and ray tracing models. The thermal model consists of thermal resistance and heat transfer models. The APIs for both optical models (Mie and ray tracer) were published under Apache 2.0 license on GitHub. Scripts for running the optical models via MuPIF JobManager were developed, as well as for running a single instance of the model with or without NAT (Network Address Translation) or SSH tunnel. The distributed

simulation runs covering all optical and thermal models were successfully run, also presented during the 3rd MMP Webinar and in CECAM plug fest held in Dublin, 2016.

The second test case was WP3 on CIGS thin film selenization process modelling (see also section 3.3), where a linking of the CFD macro simulation using X-Stream software (Celsian Glass&Solar B.V.) and the micro structure evolution simulation using MICRESS (Access e.V.) is used, supported by an additional model to evaluate quality factor of a CIGS film, based on microstructure properties - e.g. average grain size, phase fractions. Both software packages (X-stream and MICRESS) have been integrated in the MMP platform's execution model, i.e. input modification, steering, and result collection can be done locally or remotely on execution servers through their application interfaces. Due to the high numerical demands, an elaborated simulation setting was used, taking the advantage of parallel execution X-Stream application and concurrent execution of individual microstructure simulations on a computer cluster, i.e. steering a larger number or even all simulation together depending on the compute resources. The first simplified simulation scenario have been successfully demonstrated during the 3rd MMP webinar. The more elaborated scenario was presented at the CECAM plugfest in Dublin in September 2016. First tests with automatic optimization have been done in the second half of the project.

In its final release, the MuPIF platform has reached TRL5. It has been tested in realistic industrial environments, where prototype simulation chains have been executed in a distributed configurations set up by the project. The MuPIF platform is distributed as open-source, under LGPL license. The MuPIF website is maintained at hppt://www.mupif.org, source code repository is hosted at Sourceforge, and the installation packages are regularly released via Python Packaging Index.

Scalability

The platform scalability depends on the scalability of the used software programs in the simulation chain. The participating MuPIF modules and their efficiency of handling data (esp. big data if problem sizes are getting larger) and exploiting the capabilities of the external software packages are limiting the scalability of the platform.

There are strategies for parallel field mapping in MuPIF, published B. Patzák, D. Rypl, and J. Kruis. Mupif – a distributed multi-physics integration tool. Advances in Engineering Software, 60–61(0):89 – 97, 2013. Some simulation workflows are naturally asynchronous, like in WP3, where RVE simulations can be performed in parallel. The platform can exploit this parallelism, the efficiency depends on load balancing of these individual simulation, in general the more simulations to be performed allows for flexible load balancing and therefore leads to better scalability.

Regarding the scalability of X-stream: The parallellisation of X-stream is based on dividing parts of the geometry over a number of processors. If neighbouring parts of the geometry are located on different processors, communication between the processors is needed to exchange the solution over the boundary between neighbouring parts. Also, the solution of the discretised Navier-Stokes equations is based on an iterative method. This means that each processor performs 1 iteration for all geometrical parts on this processor. A smart algorithm is used to divide the geometrical parts over the processors, however the geometrical parts will never be exactly equally divided over the processors. As a result at the end of a iteration, the processors have to 'wait on each other' till all processors have finished this 1 iteration. Than all processors can start the next iteration.

Summarizing, there are 2 factors influencing the scalability of X-stream with the number of processors: the communication overhead between processors (influenced by the division of the geometry over the processors and dependent also on the communication speed of the used computer/processors/network) and the division of the geometrical parts over the number of processors used (influenced by the set-up of the grid and the physical models applied in the simulation). Therefore, the scalability is case- and computer dependent. In a test performed to judge the scalabity of GTM-X a linear scale-up with number of processors was observed up to 16 processors. For higher number of processors the communication overhead increased too much, reducing the scale-up.

1.3.3 Case study: phosphor converted lighting systems

The main scientific and technology result of WP2 case study is the developed opto-thermal multiscale modelling scheme to solve the design optimization problem using phosphors as light conversion material. This simulation scheme and its data flow are depicted in Figure 4. In the figure, the blue boxes correspond to the models, green boxes input/output data generated by the models, and grey boxes the end user interaction (input data for the models, output data from the models).
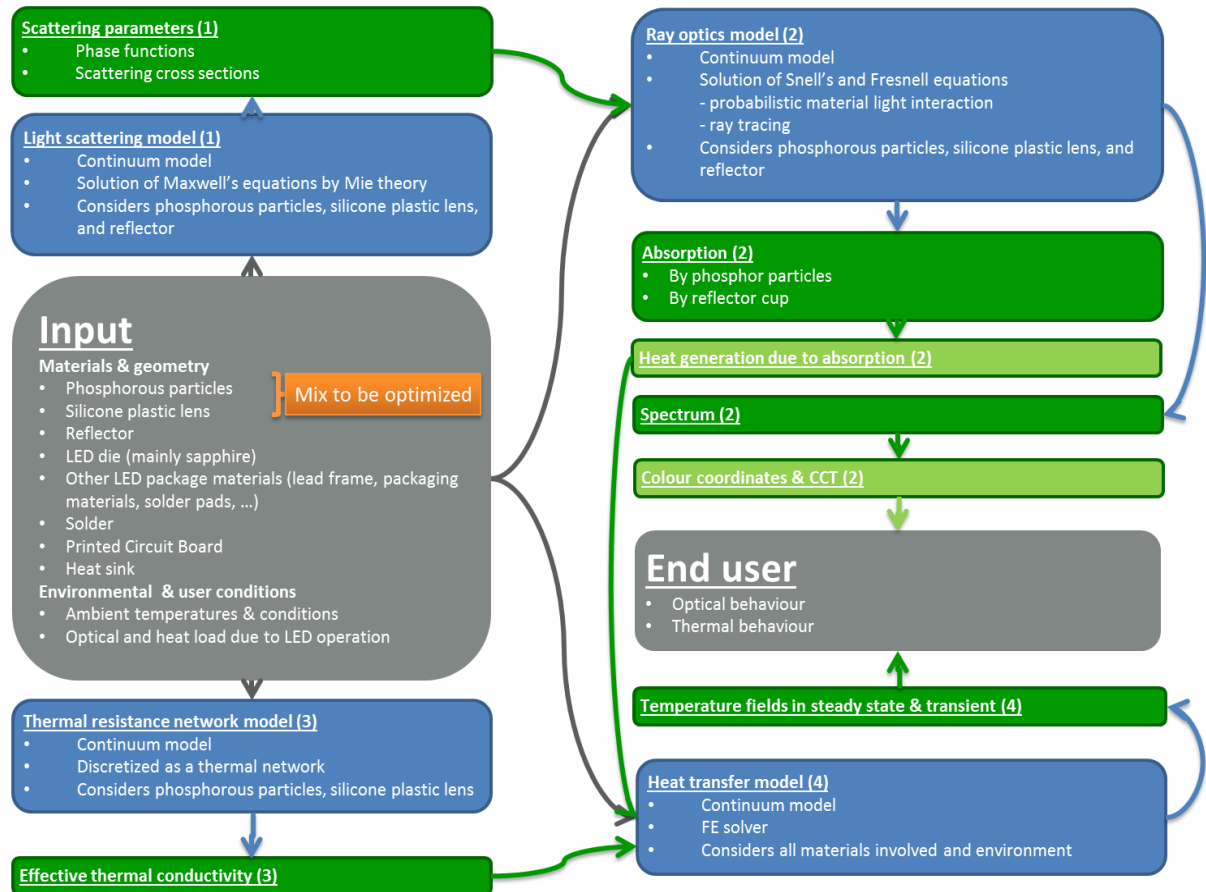
Figure 4. Simulation scheme and the data flow

The optical model consists of two models: light scattering model based on Mie theory calculates the scattering probabilities and scattering angles which are needed to obtain the ray path lengths. The ray optics model uses ray tracing to calculate the angle dependent spectrum (wavelength, intensity), and the thermal absorption of the LED phosphor material. From the obtained spectra several optical characteristics such as colour correlated temperature (CCT) and colour coordinates can be calculated. The thermal absorption is used as an effective heat source in the thermal model. The thermal model consists of two submodels: the thermal resistance circuit (TRC) model which computes the effective thermal conductivity in the silicone plus phosphor mixture, and a continuum model of the LED package that provides the stationary temperature distribution inside the entire LED and the transient temperature distribution during cooling down. These transient cooling curves can be used by the end
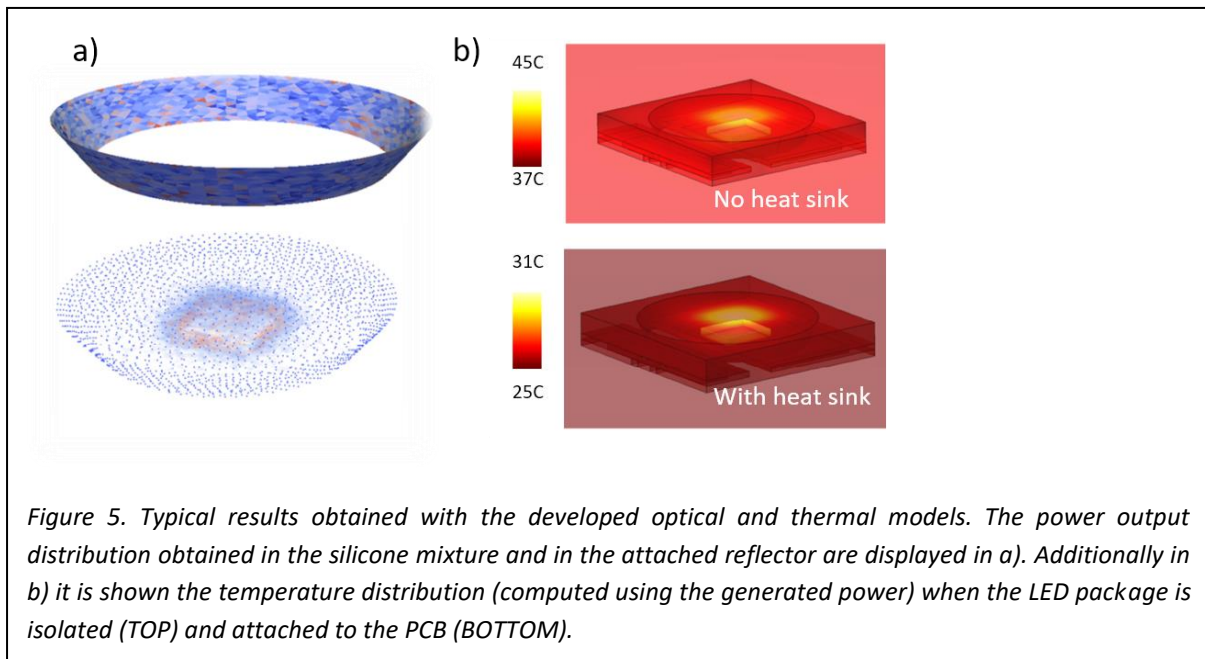
user to derive structure functions (thermal resistance/capacitance map), which provide information about device reliability.

Originally, an optical-thermal coupling was envisaged, as excitation, absorption and emission spectrums of phosphor materials are temperature dependent. Therefore, the colour correlated temperature (CCT) of the LEDs also changes with temperature. However, the required operation temperature of LEDs is within a small range. Within this temperature range, there is no relevant temperature dependency. Therefore, it was decided to neglect the optical-thermal coupling.

The Mie scattering model is implemented in Python, the ray tracer in C++. The thermal submodels are written either in Matlab or COMSOL. In order to connect all the models, the MuPIF platform was used. For that, MuPIF APIs were implemented in Python for all the models. The optical models and their MuPIF APIs are published as open source software under Apache License, Version 2.0. The codes are available in GitHub:

- https://github.com/ollitapa/VTT-Raytracer

- https://github.com/ollitapa/MMP-TracerApi

- https://github.com/ollitapa/MMP-MieApi

Figure 5. Typical results obtained with the developed optical and thermal models. The power output distribution obtained in the silicone mixture and in the attached reflector are displayed in a). Additionally in b) it is shown the temperature distribution (computed using the generated power) when the LED package is isolated (TOP) and attached to the PCB (BOTTOM).
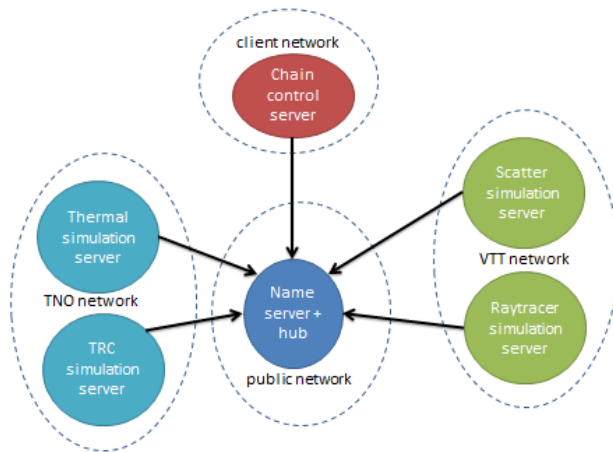
Figure 6. Implemented nameserver+hub approach (left) used to run the simulation chain over different corporate networks. The black arrows represent the instantiation of connections, which is always from corporate network to outside, never reversed. The data flow will be bi-directional as soon as the connection is established.

One of the key features of MuPIF is that it makes possible for the simulation codes to transfer previously standardized data across different computers. In the case when all computers utilized for this purpose are located in the same internal network, configuration of the platform is straightforward. However, achieving the same degree of success for a platform configured among different corporate networks is more cumbersome because of strict IT security policies of each company.

Therefore, for running the developed simulation chain, we used the setup depicted in *Figure .* This approach is based on a separated computer outside all corporate networks that acts as a nameserver+hub. Since it is located in a more flexible network, it is able to accept connections from other computers all over. Additionally, the data traffic could be safely routed by using SSH tunnels. In order to avoid having an "open door" in the system, access was limited and controlled:

1.   Only a limited set of IP addresses or ranges are given connection permission to the nameserver at a single port. These IP addresses are provided by the simulation chain participants.

2.   All connections are SSH encrypted and the encryption keys are provided by the simulation chain participants.

3.   The simulation chain will not start until all simulation chain participants have started their simulation server and the secure connection to the nameserver+hub is established. If for whatever reason a participant does not trust the connection it can stop the connection to the nameserver, which stops any traffic.

An additional advantage of having such a common resource outside the corporate networks is that different parties do not share key information in between them. The only connections made are to the nameserver+hub and not between each other networks. However, there exists the possibility to connect the applications directly if necessary. In this way, the data transfer can be made much faster, which may be desired when transmitting large amount of information.

It is important to mention that the challenges faced in configuring the simulation chain among various companies are due mainly to corporate IT policies. These challenges contrast with the simple configuration and use of the platform itself. It is also to be noted that this is not the only possibility to setup the system. For example, we have also used a setup, where the nameserver was running in VTT's server together with the optical models. In that case, the optical models could be connected to the nameserver without SSH tunnels thus without any encryption.

The simulation chain was then used for demonstrating LED design optimization. For the optimization target, we chose the CCT of different phosphor mixtures, i.e. what are the optimal weight fractions of green and red phosphor particle types in order to obtain light out of a given CCT in black body locus. In general, our optimization strategy is based on a brute force method: the LED design space is explored by simulating in a limited number of grid points for selected system parameters. In order to save time, the values between the simulated points are interpolated. Finally, the global minimum (or maximum, depending on the optimization target) value for the merit function is searched using the interpolated values. Since interpolating may cause some inaccuracy in the values, the optimization routine can be iterative. The surroundings of the found global minimum/maximum point can be explored again using a smaller step between grid points. The optical model is based on statistical behaviour and this causes also some variation in the individual simulation runs. This can be minimized by using the average values from several independent simulation runs.

In our example case, we calculated the colour coordinates corresponding to the targeted CCT in black body locus and then used the Euclidean distance from the targeted coordinates to the simulated coordinates as a merit function (see Figure 7). The global minimum for the merit function was searched by using a basin-hopping algorithm. Running the simulation chain with the found weight fractions gives finally the resulting CCT (see Figure 8), colour coordinates, LED spectrum, etc.

The simulation results were validated against manufactured samples. The resulting trends from the experiments were captured by the model simulations. Discrepancies were initially observed and it has been shown that adjusting of key parameters in the model, such as the phosphor efficiencies, improve the accuracy of the results. As a conclusion, the optimization of phosphor-based white LED package design is possible with the MMP simulation chain, starting from a well-known design that can be used for calibration.
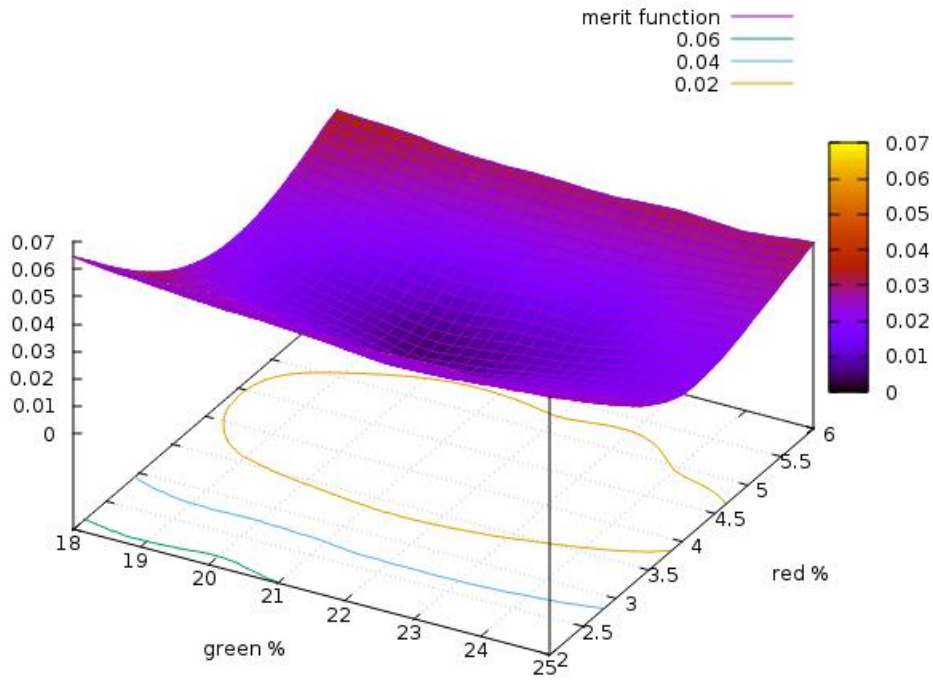
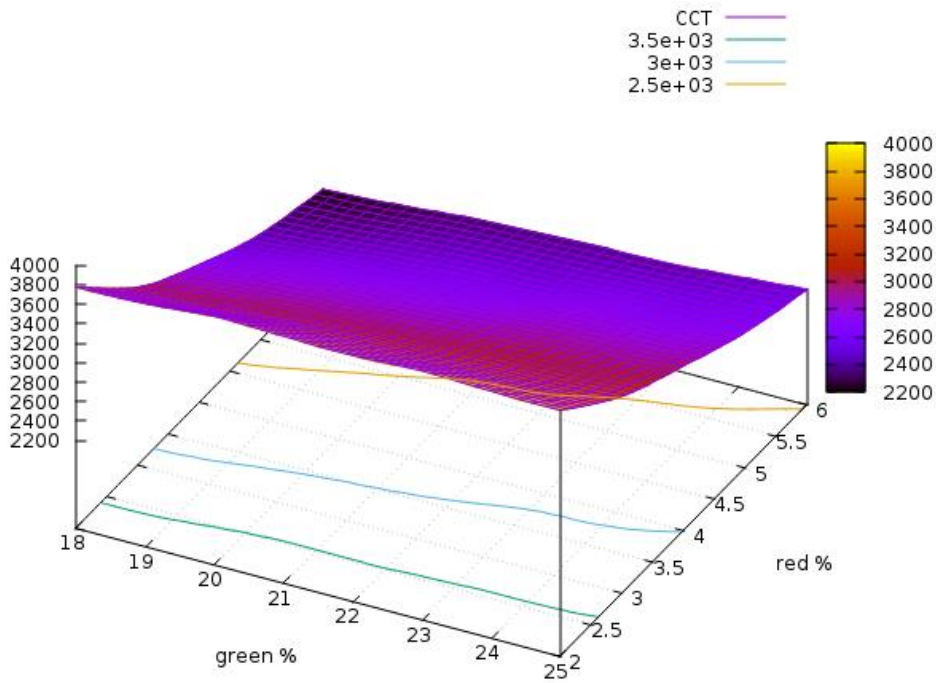*Figure 7. Example merit function. The minimum in (21.4%, 4.1%) gives the optimal weight fractions.*

Figure 8. Example CCT values as a function of weight fractions

1.3.4 Case study: CIGS process optimization

Both case studies have two different aspects. At first they are considered generally for the development, testing and demonstration of an industrial relevant demonstration example for the multiscale modelling platform MuPIF and secondly they should contribute to a deeper fundamental understanding to the processes under consideration and thus eventually lead to process improvements. In the CIGS application, the target is the quality improvement of CIGS thin films fabricated via selenization meaning improved film quality for solar cell applications.

To meet the objectives, it was necessary to develop the complete modelling chain, in particular CIGS specific material models and CFD based thermal furnace models comprising the special features of the selenization furnaces, e. g. including Selenium evaporation. Also, there was a need for the development of a dedicated quality criterion as the production of solar cells itself was not part of the project. Material characterisation was intended to calibrate and verify the modelling results.

The status at the beginning of the project can be summarized as follows:

- Thermodynamic CALPHAD-databases: A thermodynamic model was only available for the ternary system Cu-In-Se (including the three binaries). Thus, neither a thermodynamic database including Ga and the target phase CIGS was available nor the relevant metal Mo was included which is important to include the reaction of Se with the metallic back contact. A literature survey showed that sufficient experimental data was available to attempt a comprehensive thermodynamic modelling of the Cu-In-Ga-Se-Mo five component system.

- No macroscopic thermal furnace was available. The thermal behaviour of the different furnace designs used for processing, in particular the transient behaviour during change of temperature settings and the evaporation of Se was weakly understood. Three different furnace designs where under discussion: i) lab scale tube furnace, ii) RTP furnace and iii) an industrial scale selenization furnace with different heating zones.

- A 1D reaction/diffusion model describing phase formation and reactions in the Cu/In/Ga metallic precursor film was available at TNO. No 2D or 3D microstructure simulation model was available at the premises of the partners nor reported in the literature. The phase-field model and the software code MICRESS, both developed at ACCESS had been successfully applied to multicomponent metallic alloys but never before to chalcogenide systems with numerous compound phases or phases with complex lattice structures and corresponding, complex sublattice models.

- A rough qualitative understanding of the impact of different microstructural constituents (e. g. binary phases, film thickness …) on the quality.

In summary, the development of a complete new simulation chain for the selenization process was necessary. The workflow of the targeted simulation chain is given in Figure 9 in the MODA style:
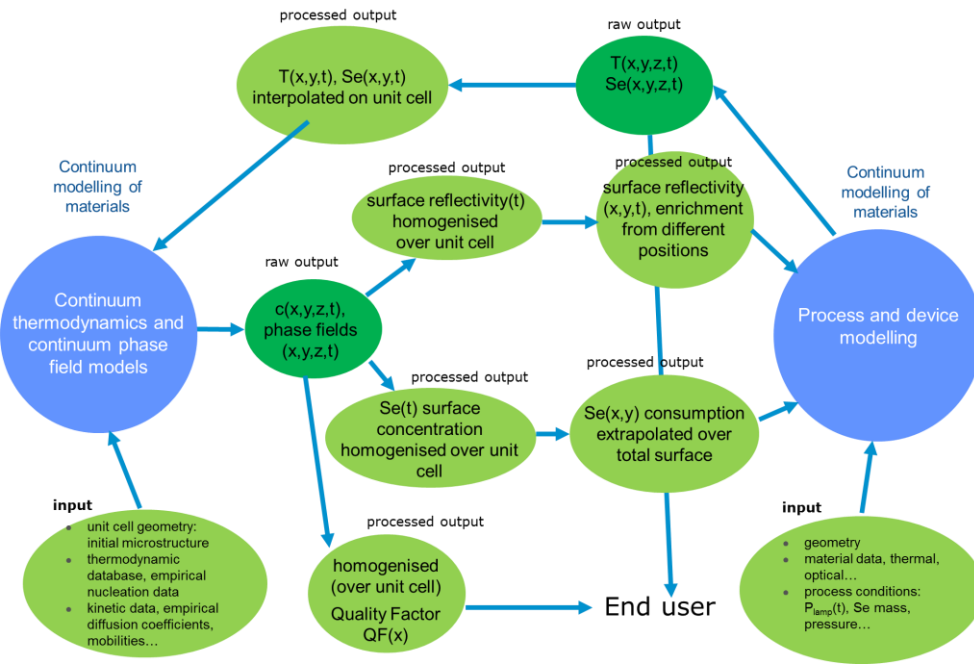
Figure 9: Workflow of the simulation chain for the selenization process.

The goal of a comprehensive quantitative simulation of the CIGS formation could not been reached completely within the project, but significant progress could be made in many different aspects:

- A complete CALPHAD description (continuum thermodynamics) of the Cu-In-Ga-Se-Mo five component alloy system has been developed which allows quantitative computations of phase equilibria, driving forces or equilibrium phase compositions. Figure 10 shows a few computation examples. The results are showing the thermodynamic equilibrium state and provide the sound basis for any kinetic modelling.
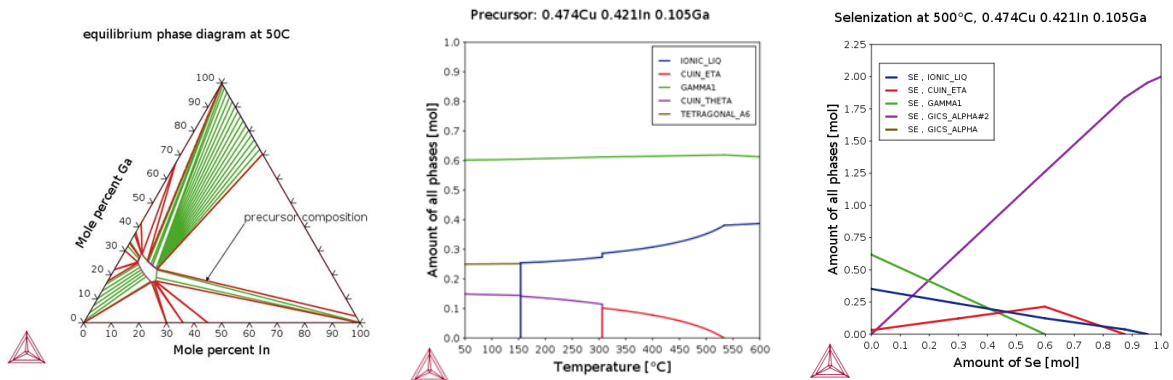
Figure 10a: Ternary Cu-In-Ga phase diagram at 50°C. The arrow marks a typical integral composition of the initial precursor film.

Figure 10b: Equilibrium phase fraction versus temperature for an In rich precursor film with a fixed ratio [Ga]/([Ga]+[In]) = 0.2.

Figure 10c: Selenization of the precursor film (equilibrium), adding Se while keeping the amount of other elements fix.

- Macroscopic thermal models (process and device modelling) have been developed for three different furnace types including the RTP concept followed by Abengoa and the industrial scale selenization furnace operated by Solliance. All three models have been calibrated and thermal simulation results have been quantitatively compared with measurements at the real furnaces. This comprises also measurement of emissivity data for the CIGS thin film, a quantity which is important to compute the radiative energy transfer especially for the RTP process. In conclusion, validated thermal process models are available which already delivered new insight into the thermal behaviour of the Solliance furnace. In future, the models can be used straight forward to investigate the effect of modified process parameter on the temperature distribution in the furnace and the transient thermal history of the substrates.
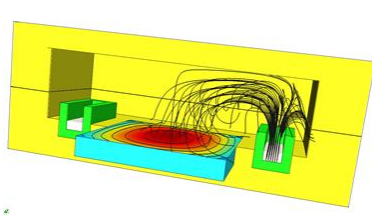
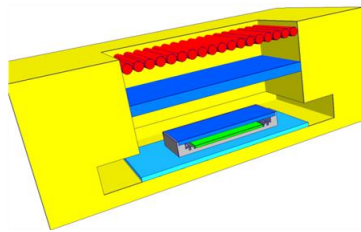*Figure 11a: Thermal process model of a tube furnace assembly for selenization (batch process).*

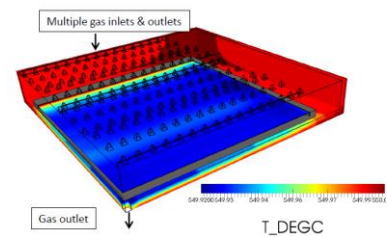*Figure 11b: Thermal process model of RTP furnace.*

Figure 11c: Glass substrate as part of the selenization furnace operated at Solliance.

- Phase field models with different levels of complexity have been formulated and numerically tested. It turned out that a quantitative model fully coupled to the thermodynamic database was numerically unstable and therefore could not been used for simulations. Within the project, it was not possible to trace back the numerical problems to a single reason. An important issue is certainly the fact that many phases in the Cu-In-Ga-Se system have a rather complex thermodynamic description, e. g. dedicated sublattice models characterised by very limited solubilities of certain elements or showed strong demixing behaviour upon temperature change. For deviations from equilibrium compositions driving force computations then often diverge or the local equilibrium calculation jump between different local minima which makes simulations impossible. Therefore, different simplifications have been attempted, e. g. a mixed thermodynamic material modelling combining a CALPHAD description with linearized phase diagram approximations. Also these simplifications suffered from numerical problems, partly due to the fact that the selenisation process covers a wide temperature range from room temperature up to 550°C and a wide range of the Se content from 0% to 50%.
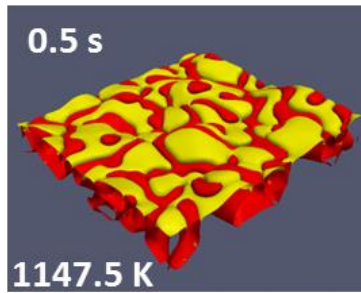
Figure 12a: Fully thermody- namically coupled simulation of δ-CuInSe2 (yellow) and β-Cu2Se (red) growth from a Cu-In-Se melt.
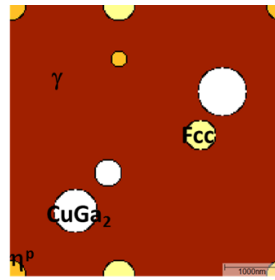
Figure 12b: Initial micro- structure of a Cu-Ga-In precursor film (with fcc, CuGa2, η and γ-phase), combined CALPHAD description and linearized phase diagram model. Kinetic simulation of an annealing step at 200°C.
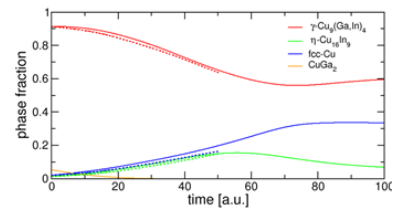
Figure 12c: Integral phase fractions corresponding to Fig. 6b. The dotted lines show results with a linearized phase diagram description compared to the CALPHAD model (solid lines).
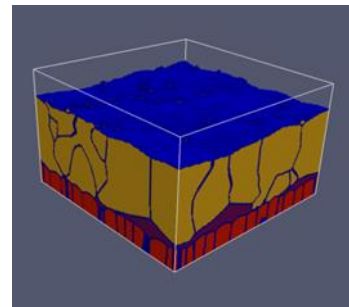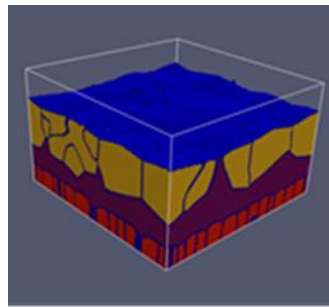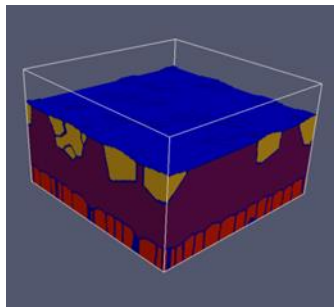

Figure 12d: CIGS formation (yellow grains) simulated with an uncoupled phase field model which does not take into account composition and diffusion. The transformation kinetics needs to be calibrated by experimental reference data. A similar simplified model has been used for the prototypic simulation chain.

- A quality functional has been developed which allows measuring the film quality dependent on microstructural parameter, i. e. dependent on the film thickness, phase amounts or grain sizes. Once improved microstructural models are available the quality functional can be used for process optimisation as it allows comparing different microstructure predictions according to their potential for solar cell properties.

- Prototypic simulation chain for testing the MuPIF platform. Despite the limitations of the microstructure models for transformation of the precursor film into CIGS, a simulation chain have been composed which comprises all necessary models and mimics all data flow according to the graph shown in figure 3. In particular, the simulation chain combines the software X-Stream for the thermal simulation, the phase field software MICRESS for the microstructure simulation, a platform service for the computation of the quality factor and homogenisation of the results (interpolation of local information over the whole substrate). Emissivity data are taken from a look up table according to local thin film composition. The prototypic simulation chain proofs that all necessary platform elements are in place and operational, thus the platform itself is applicable for the selenization process. Quantitative

and predictive simulations are thus only a matter of the further improvement of the individual models and do not require much effort in the platform development.
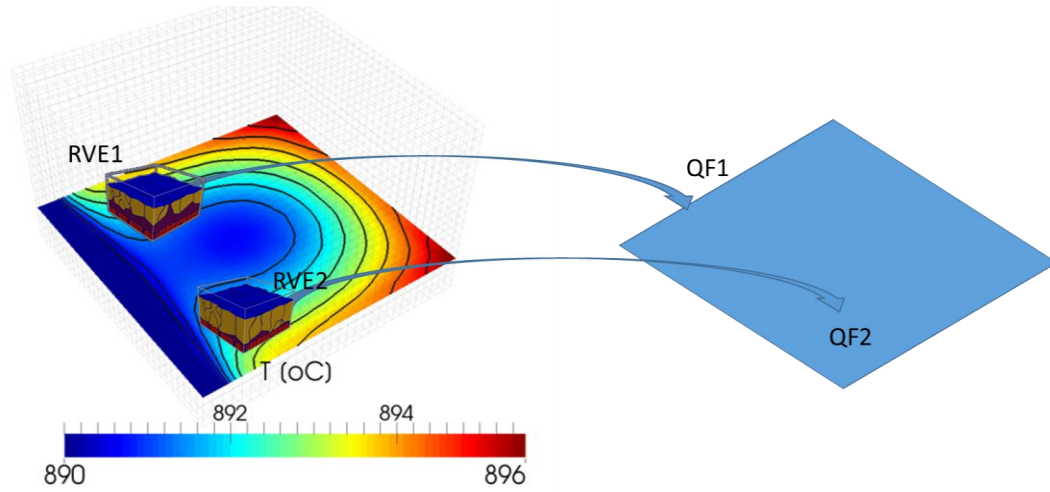

Figure 13: Schematic figure of results obtained from a coupled multiscale simulation (prototypic simulation chain). Shown on the left is the temperature distribution over the substrate (macroscopic process simulation) together with two different RVE's for microstructure simulations. The quality factor is evaluated for the individual RVE's and mapped back on the substrate. Interpolations between different local computations allow obtaining the quality factor at any location on the substrate. For the present geometry around 25 local RVE's are needed for a sufficient interpolation.

Mathematical equations and numerical methods

We have used a general multi-phase field (MPF) model framework for the microstructure modelling. The underlying model and related equations are published e. g. in J. Eiken, B. Böttger, I. Steinbach: Phys. Rev. E 73 (2006), 066122 and B. Böttger, J. Eiken; M. Apel, Computational Materials Science Vol. 108, pp. 283-292 (2015). In the MPF model the evolution equation of each entity, e. g. the dual interface an individual grain of a particular phase is descried by an equation of the type

$$\dot{\phi}_n = \mu_{ij}\left\{ \sigma_{ij}\left[\nabla^2\phi_n - \frac{\pi^2}{2\eta^2}\left(2\phi_n - 1\right)\right] + \frac{\pi}{\eta}\sqrt{\phi_n\left(1-\phi_n\right)}\,\Delta G_{ij}(T, c_\alpha)\right\}$$

Here, $\phi_n = \phi_n(t,x)$ is the phase field related to grain n, μ_{ij} and σ_{ij} are interface mobility and interfacial energy which could be a grain or phase boundary energy dependent on the type of dual interface. Please note that in the MPF framework each individual grain is described by an individual phase field, thus a simulation can easily lead to a set of about 100 phase field equations. μ_{ij} and σ_{ij} comprise all possible phase interactions and grain boundary energies. The parameter η is the thickness of the diffuse interface and can be chosen as 5 grid cells for numerical convenience. Finally, ΔG_{ij} (T, c_α) is the temperature and composition dependent local thermodynamic driving force which is computed either by (i) a local quasi-equilibrium computation based on thermodynamic databases, by (ii) a linearized phase diagram approximation or (iii) stated as constant in the prototypic simulation model. Interfacial mobility has been qualitatively adjusted in a way that the computed transformation kinetics corresponds to the experimentally observed time scale for the selenization process. The interfacial

energies have been set to a constant value of 10^{-5}J/cm^2 which could be considered as an educated guess. Both quantities could be in future derived from first principle DFT or semi-empirical force field methods. So far, no results from atomistic simulations have been reported in the literature.

For the modelling based on (i) and (ii) diffusion of all elements is computed based on Fick's equation:

$$\dot{c}_\alpha(x,t) = \nabla \cdot \sum_p \phi^p D^p{}_\alpha \nabla c_\alpha$$

with c_α the composition field of element α, $D^p{}_\alpha$ the diffusion coefficient of element α in phase p.

The phase field and diffusion equations are solved by finite difference discretization in a forward Euler scheme.

As initial condition a microstructure representation of the precursor stack has been used. This has been done by creating synthetic microstructures of different levels of complexity, from homogeneous thin films to multicrystalline structures.

Boundary conditions are periodic in the x-y-plane and adiabatic on top and bottom. For model variants (i) and (ii) Se concentration on the top side has been set via a Dirichlet condition. Temperature is superimposed over the whole domain with values taken from the macroscopic furnace simulation.

1.4 Potential impact

1.4.1 Strategic impact

More and more products benefit from nano-scale properties and nano-scale material phenomena in order to improve their performance or to acquire new functionalities. The development of nano-enabled products and processes is strongly multidisciplinary. At present, each of these disciplines develops and applies primary their own modelling software tools. For example, in optics, ray tracing packages like Zemax and LightTools are used, where thermal and structural modelling mainly uses Finite Element tools, like Ansys and Abaqus.

In order to challenge nano-engineering problems, the mutual coupling of these modelling resources is required. For this reason the MMP project partners have developed a multi-scale and multi-physics simulation platform (MuPIF), which provides a flexible, modular, and interactive scripting environment, with distributed and parallel processing support. The MuPIF platform can be of great help on enabling integrated simulations of manufacturing processes and product performance. Through the possibilities of this multiscale modelling platform, the design of these products and related manufacturing processes will create a thorough understanding of the interactions between nano-, meso- and macroscale properties and physical phenomena between scales. The power of MuPIF is its generic nature achieved by the Application Programming Interface, the open access of the developed MMP-platform and possibility to plug-in commercial codes without violating IP right, which is made possible by the GNU-LGPL open source license.
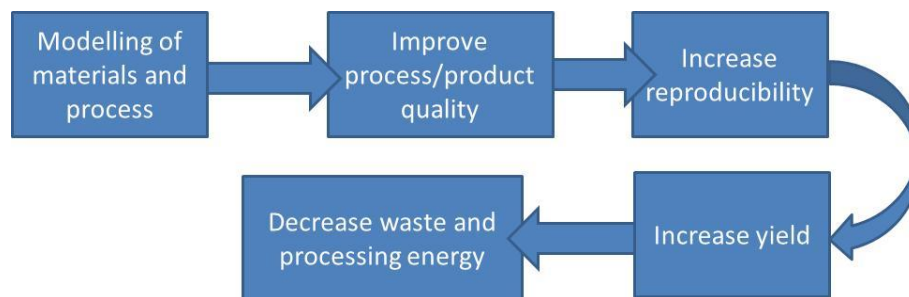

Figure 14 Impact of full modelling of materials and production processes.

Integrated computational materials engineering (ICME) is already an accepted method in the development of mechanical structures, e.g. aluminium casting for engines, and other mechanical applications. In those fields development times are reduced from a normal 10-20 year period to 2-3 year period. MMP went beyond ICME by extending the possibilities to other high-tech applications with other physical properties and processes, from nano to macro scale.

1.4.2 Selection of use cases

The MMP consortium has taken the markets and technologies identified in the NANOfutures roadmap[1] as the starting point of the selection of the use cases. NANOfutures, a European Technology Integrating and Innovation Platform, identified multiscale-multi-physics modelling as one of the major drivers to exploit nanotechnology to its full potential in the following lead markets:

- In energy for energy generation, harvesting, storage and distribution needs (high barrier properties for energy cell, enhances gas absorption and trapping, efficient transmission, magnetic storage);

- In ICT, especially nanoelectronics and photonics, in multilayers , porous structures and nano-structures and their integration;

- In building and construction to improve aesthetic, optical, mechanical, durability, safety properties of building materials and components;

- In medicine and pharma for regenerative medicine, diagnostics and drug delivery.

Two economically relevant cases have been selected out of these identified markets: LED lamps and CIGS based thin film photovoltaics.

Use case: phosphors in LED

It is forecasted that the worldwide lighting market will grow to EUR 110 billion in 2020 and it is expected that close to 60% of the overall lighting market in 2020 will be LED lighting. The current size of the global lighting market is EUR 69 billion, of which EUR 7 billion are contributed by LED (about 10%). The market of the case study of solid state lighting is led by European companies, but competition from mainly Asian companies is closing in. The global lighting market reached a €58 billion turnover at 2009 and it is expected to grow to approximately €180 billion at 2020 (see Figure 15). The demand of LED packages will grow from 3.3 billion units in 2009 to 30 billion units in 2020.

Figure 15 Global solid state lighting (SSL) market forecast 2020.

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[1] NANOfutures Integrated Research and Innovation Roadmap (2013-2025), 2012
http://www.nanofutures.info/sites/default/files/NANOfutures_Roadmap%20july%202012_0.pdf

A sharp decrease in costs of about 30% p.a. in the next ten years should lead to an increase in market share for LEDs from the current 10 to the anticipated 70% in 2025 (see Figure 16). In face of strong global competition to benefit from this growth, it is essential that European developers and manufacturers reduce lead time and development costs of their new products and bank on cost reduction and performance improvement potential of new nano-technologies.

The software platform that has been developed within the MMP project can contribute to this, by connecting the effect of the new technologies and materials to the performance of the total device. Through the multi-scale approach offered by MMP optimisation of the full system of LED is achieved. The size of this market is 206 billion Euros in total.
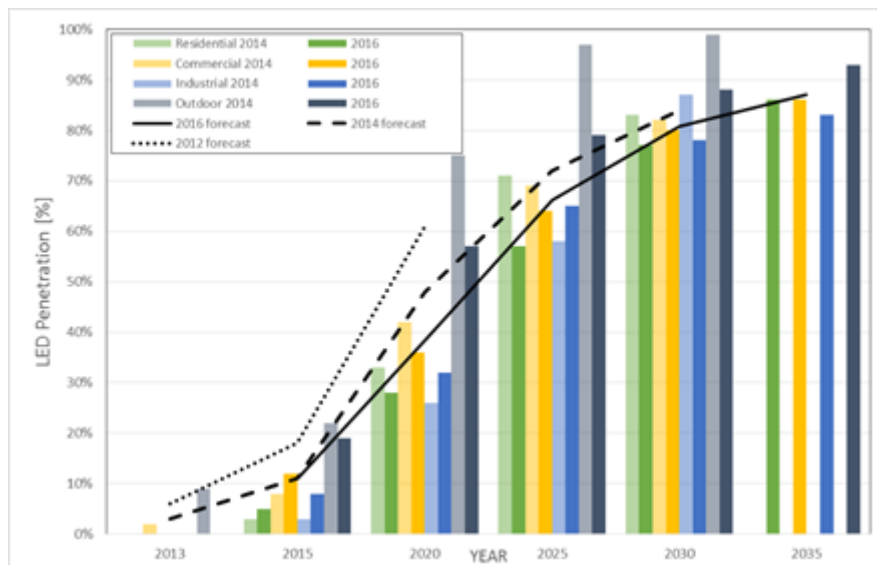

Figure 16 LED penetration levels in four applications, blue line indicates overall trend (DOE data from [2,3], 2012 data from [4] ; with permission).

By enabling an efficient design of LED lamps and LED luminaires, the MMP project will have a clear influence on the environmental effects of the production of this type of lighting, which is in itself already a very efficient light source. The platform developed in MMP will enable to decrease the time to design and time to market of novel products. Also less energy is needed for experimentation and both energy efficiency in production as well as efficiency of the product can be optimized. Detailed prototyping, light output, thermal efficiency, and hence reliability will be optimized for the requirements of specific applications.

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[2] Navigant Consulting, Inc., Energy Savings Forecast of Solid-State Lighting in General Illumination Applications, report prepared for the U.S. Department of Energy, August 2014.

[3] Navigant Consulting, Inc., Energy Savings Forecast of Solid-State Lighting in General Illumination Applications, report prepared for the U.S. Department of Energy, September 2016.

[4] Estimated LED penetration of the global lighting market from 2010 to 2020, available at http://www.statista.com/statistics/246030/estimated-led-penetration-of-the-global-lighting-market/ (last visited on 8/25/2016).

Use case 2: CIGS production

The CIGS technology is an upcoming market (Figure 17). In December 2012, Lux Research presented a study stating that CIGS has the highest cost reduction potential of all PV technologies, making it competitive with the other leading technologies by 2016. MMP will contribute to make the European CIGS activities cost competitive.

The current size of the global PV market is 67.4 GW total installed capacity of which 27.7 GW has been installed in 2011. 70% of the global PV market is located in the EU. The photovoltaics (PV) market will be twice the size in the coming 4 years, to have 60 Gigawatt installed peak power. The total global market leadership in 2007 was still in hands of Europe (32%), but China and Taiwan have become market leaders with a share of 54% in 2010 [5]. Mostly this concerns first-generation silicon wafer-based modules which have by far the largest share of the PV market at this moment (market share of 87%).

The MuPIF platform has the potential to enable material improvement of CIGS by the integrated approach of process simulation and microstructure simulation. The platform technology supports CIGS development and thereby, it can help to enable Europe to regain market share in the photovoltaics industry. Every 1% in absolute improvement of solar module efficiency by improved industrial processing corresponds to a market value of about 350 M€. Control of crystal growth of the CIGS layer itself is one of the most important factors for this improvement.

In CIGS production, a higher yield amounts to a lower cost of the panels as well as less scrap. The process itself can then contribute to a higher sustainability. Through cost of ownership modelling a with a theoretical yield of 96% for the three processes involved in the executed simulations, a 250 MW CIGS factory would end up with a total yield of 82.6% (other processes are also not at 100% yield). An increase of these processes to 99% would result in a total yield of 90.6%. The theoretical cost of non-yield is decreased with 50%, from 16 million Euro to 8 million Euro. Optimisation of the process using the MMP platform and the appropriate models will therefore lead to saving of costs, which in turn make the products competitive.
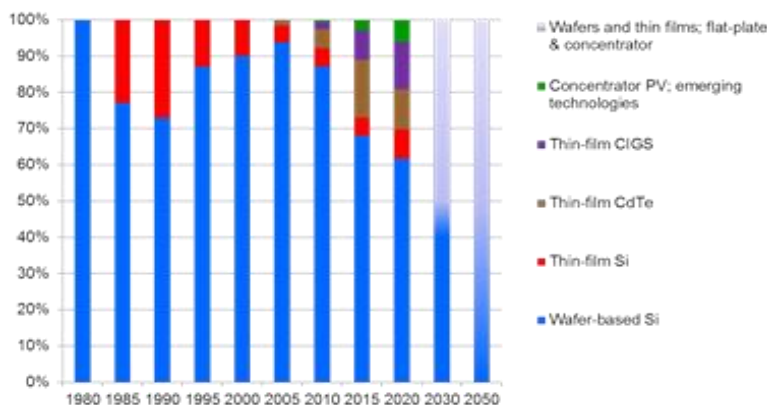

Figure 17 Relative market share of PV technologies. From: EPIA Solar Generation 6 (Issued 2011)

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[5] "A strategic research agenda, 2nd edition", 2011, Photovoltaic Technology platform, European Commission.

1.4.3   Dissemination & Exploitation

To achieve the impacts mentioned above, the MMP project has disseminated the project results through workshops at conferences, which have also been published through the Wiki page (www.mmp-project.eu). The Wiki page also serves to connect other user groups to the platform and involve software developers. The source code has been published under an Open Source public license (GNU Lesser GNU Public License (LGPL)) that allows a broad distribution of MMP, but protects the intellectual property encoded in the glue code and service modules. The license also facilitates 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.

The cloud architecture developed in MMP makes it possible to explore alternative business models for software modules. For example paying for the time of using software modules instead of buying them.

Recorded webinars, publications and other public results can be found on the website: www.mmp-project.eu

A major concern of the MMP consortium is to maintain and increase the community using the MuPIF platform. Therefor the targeted website www.mupif.org has been launched, which will continued to be used by project partners in follow-up projects. Further promotion of the platform will be performed in cooperation with the ICMEg foundation.

CTU will maintain and further develop the platform at least for the next 4 years. The part of this commitment is to provide (non-commercial) support via the MuPIF and sourceforge websites. As the MuPIF is been in new EU project (Composelector), the dissemination on MuPIF platform will naturally continue in frame of this project, as well as in frame of ICMEg and EMMC where CTU actively participates.

1.5 General project data

A list of all beneficiaries with the corresponding contact names is presented in the following table.

No	Beneficiary	Type	Ctry	Contact person(s)	E-mail
1	Nederlandse organisatie voor Natuurwetenschappelijk onderzoek - TNO	RTD	NL	Sjoukje Wiegersma Dorrit Roosen Fidel Valega Mackenzie	sjoukje.wiegersma@tno.nl dorrit.roosen@solliance.eu fidel.valegamackenzie@tno.nl
2	Technische Universiteit Eindhoven - TU/e	Univ	NL	Mark van den Brand	m.g.j.v.d.brand@tue.nl
3	Ceske Vysoke Uceni Techicke v Praze - CTU	Univ	CR	Borek Patzak Vit Smilauer	borek.patzak@fsv.cvut.cz vit.smilauer@fsv.cvut.cz
4	ACCESS e.V. - ACCESS	RTD	GER	Markus Apel Ralph Altenfeld	m.apel@access-technology.de r.altenfeld@access-technology.de
5	Teknologian Tutkimuskeskus - VTT	RTD	FI	Aila Sitomaniemi	Aila.Sitomaniemi@vtt.fi
6	CelSian Glass & Solar BV – CelSian	SME	NL	Adriaan Lankhorst Luuk Thielen	adriaan.lankhorst@celsian.nl luuk.thielen@celsian.nl
7	Philips Lighting B.V. - PHILIPS	IND	NL	Annemieke Wondergem-de Best	a.w.m.de.wondergem-best@philips.com
8	Abengoa Solar SA	IND	ES	N.A.	

- Project website: www.mmp-project.eu

- Platform website: www.mupif.org

- ICEMg website: www.icmeg.euproject.info