

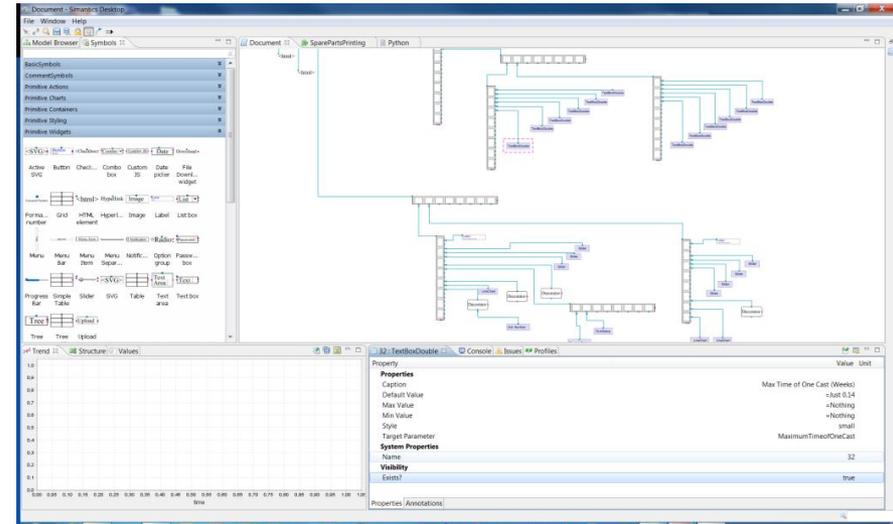
Development directions &
main achievements of the
project from viable business
model perspective

Annual e-workshop

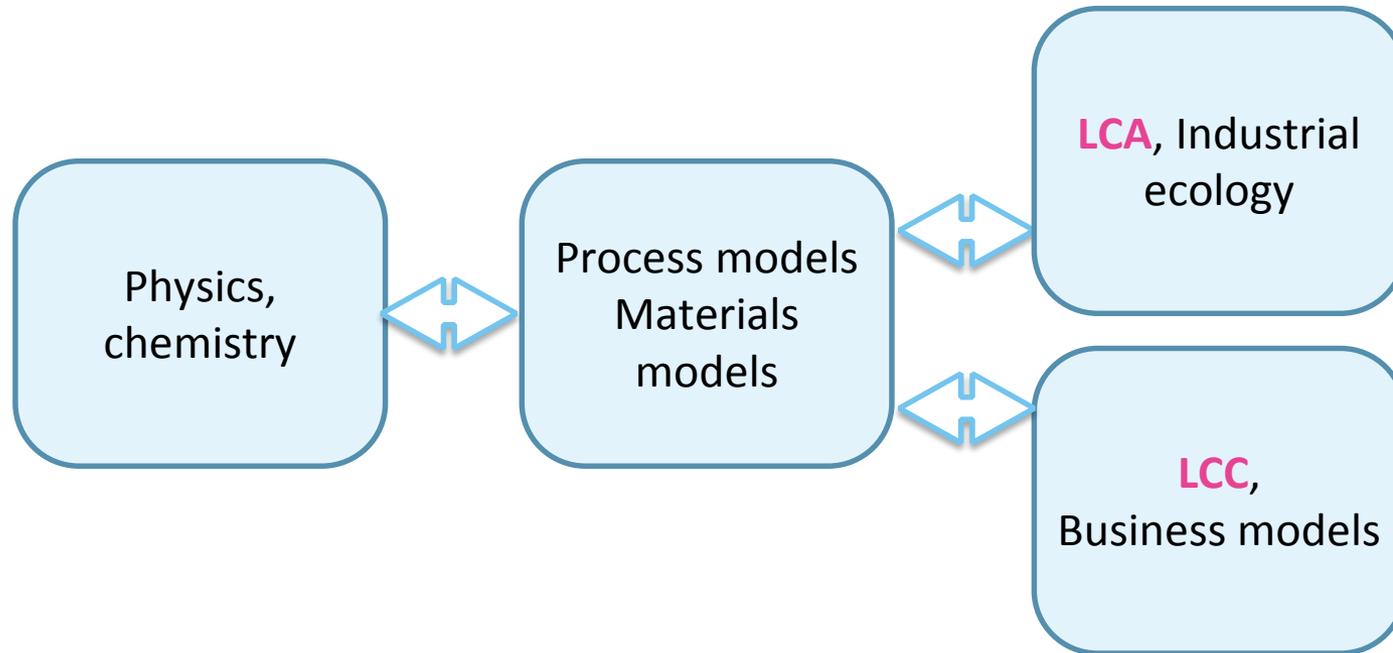
Virtual Upscaling

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Model-based Virtual Upscaling



Upscaling chains covered in the project

- There are several modeling chains (level couplings) which we have covered so far in the various WPs
- CFD – Thermodynamics/Process simulation software (Fluent – HSC-Sim)
- Direct coupling (HSC-Sim integrated into MF, Fluent communication channel exists)
- Process simulation models – Life Cycle Analysis models (HSC-Sim - SULCA)
- Both models integrated into MF
- Thermo-mechanical model coupling (Finite elem. – Finite diff.)
- Direct coupling
- Structural models – CFD (Digimat, Moldflow-Ansys)
- Direct coupling
- Thermokinetic model – System dynamic model (inhouse codes, freeware)
- Both models interated into MF (<http://modellingfactory.simupedia.com/amdh/>)

Chosen platform development directions 1

- Semantic integration platform: rapid integrations possible, **deeper integration** levels than just data integration possible
- **Various modeling paradigms and languages** can be used together
- Allow users to use their favorite tools in data production and analysis
- Not everything should be integrated: concentrate on **model/paradigm 'families'**
- Interface with HPC, do not compete with specialized solutions (e.g. support work flow management, batch jobs etc, data formats etc.)
- Support **surrogate model construction** (fast to simulate, automatable). In other words, computationally heavy models are transformed into more easily compatible fast models, which are suitable for web apps, optimization (iterative usage)

Chosen platform development directions 2

- It was not possible within the budget and the time frame of the project to integrate all software components into the platform, despite the fact that Modelling Factory does offer very flexible way of integrating different types of numerical solvers using semantic data representation as its core.
- Software licenses of proprietary codes created a challenge because in general they cannot be used *directly* in Modelling Factory type cloud services without an expensive cloud license. Therefore, open source components were preferred unless there already was a prospective business opportunity to keep using the integrated software after the project.
- In the multi-scale modeling and simulation task done in the up-scaling tasks one wishes to work with fast-to-compute models as optimization is an integral part of the design process . Therefore, it would be useful if there were a way to replace the numerically heavy models of the virtual up-scaling chain with faster versions.



Chosen platform development directions 3

- In the previous interview, the partners mentioned that integration of databanks could be one possibility, which would increase the usefulness of the platform from their point of view.
- While according to the project plan, Modelling Factory is not meant to a big data storage platform, its present implementation does provide access to various types of databanks. For example, the EcoInvent database is usable through the life cycle assessment program Sulca, which has been integrated into the platform. Also, HSC Sim Chemistry, which contains thermodynamic and process chemistry related data, has been utilized in the partner projects. However, **the databank idea can be vastly expanded by using the newly planned features of the platform, which support surrogate modeling** (see below).

Chosen platform development directions 4

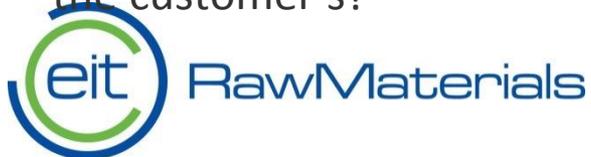
- Due to the observations on the previous slides, we adopted a new strategy emphasizing the ease of integration, speed of execution and open source features
- Computationally heavy simulation models will only be integrated if the cost-benefit analysis indicates that the job is worth the effort. **In general, we aim at using *surrogate models* in the up-scaling chains. Surrogates act as 'dynamic interpolative data banks'.**
- Surrogate modeling, of course, has its own challenges: teaching times, lack of teaching data, mastery of many (standard) techniques needed, black box

Chosen platform development directions 6

- Modelling Factory will not support **automated** surrogate production in the near future. Users wanting to utilize the platform for surrogate integration should prepare the surrogates themselves.
- The platform will only support integration for standardized surrogates belonging to certain 'families', which will be determined later (e.g. Matlab SUMO, PyBrain)). As some of these families are from IT perspective no different from models written in certain programming languages already supported by the Modelling Factory, there is in these cases no other compelling reason to produce a surrogate model from the original one besides the possible speed-up of the simulation's execution.
- The new surrogate dimension of the use profile of the platform is consistent with the wishes expressed by the partners and mentioned in the ICME part of the original project proposal of the Modelling Factory project. Many types of surrogates can be seen as dynamic interpolative databanks, which extend the idea of pointwise data storage to cover a much larger search space than in 'normal' databanks.

Questions to project partners

- Do you have any prior knowledge in machine learning or other methods, which can be used to produce surrogate models such as neural networks?
- Would surrogate/data based modeling be useful for your projects now or in the future (e.g. to be used in multiscale model chains where optimal parameter choices need to be found)?
- Does surrogate modeling create an extra burden for you (Too complicated? Too many things to be tested? Lack of skilled modelers?)
- Do you already use data-based modeling or do you plan to use it in the future in addition to 'functional' modeling?
- Do you see enough value (cost-benefit) in replacing some of the present proprietary models with open source surrogates e.g. for the purposes of disseminating your results to your customers or integrating your data with that of the customer's?



Main achievements per work package....

- Let us now move on to the individual success stories & achievements!