



Charter for EMMC team on Business Decision Support

Materials Modeling as Business Decision Support

Background

Within the EMMC subgroups have formed to focus on a certain group of stakeholders. This team focuses on business decision support systems based on materials modelling. Sustaining and growing businesses that deliver products and services meeting with the societal demands requires continuous innovation. In a global context, making well-thought out decisions on which business strategy to follow and how to best serve more demanding customers is a very complicated process. It requires making choices between multiple options both on the commercial as well as the technical side of the business. The ever growing sheer volume of information on markets in all fields of science and technology, demand a profound knowledge of the possible options open to the business for making a decision as well as insight in the consequences of a selected option. Simply stated, a business requires, at every operational level, answers to specific questions for making decisions that minimize risk and maximize the success rate of actions. In recent years, significant progress has been made in computational technologies for processing experimental and modelled/simulated data, structured and unstructured information based on algorithms for machine learning, big data handling, smart search engines, optimization, and networks, and in boosting associated hardware performance, so that data can be used in novel ways to provide customer tailored answers to specific questions. The EU Framework programs have contributed in a significant way to develop many of these computational tools in various fields. Today, it is feasible to apply the tools to process “big -science & technology and business- data” into smart options for data driven decision making that can strengthen the agility of companies, particularly SME’s.

Scope

Materials modeling, including smart algorithm development, is a leading and globally recognized competency for Europe. The academic and engineering communities have strongly invested in theoretical bases for materials models and these models are now well established in the search for new materials in a certain application domain.

The use of materials modeling in industry models in decision making requests that models provide results validated in the operational practice.

Two important challenges need to be addressed to bring materials modeling to a next level of industrial use. Easy and flexible integration of existing materials models in combination with empirical information to address various industrial problems is a first challenge. Many technical challenges have a complicated multi-variable nature. It typically requires the use of multiple models, each of which may have limited applicability or accuracy. Even then, additional empirical information is often necessary to achieve



realistic solutions to the challenge. The second challenge is the combination of simulated potential technical options with the commercial decision making process. Market trends, pricing, customer needs and demands are some of the additional criteria for selecting a specific technical solution tailored to an identified process or product need.

Accordingly the scope of the work group entails: Development and implementation of methodologies for flexible integration of various materials model types adapted to industry selected challenges that in combination with business criteria define the technically possible and commercially most attractive solution.

Participants will be industrial manufacturing companies, modellers and mathematicians.

Objective

The objective for the team is to identify, define and articulate in scope industry representative needs that enable the definition of efforts for making materials modeling an integrated part in the business decision process at all operational levels of companies. Bottom-up activities and provision of policy input to funding schemes (EU, national, international,...) will be undertaken.

Goals

1. Establish a core team
2. Define a work approach and context for addressing the defining challenges associated with the objective
3. Develop a (representative) social network on materials model based business decision support
4. Identify significant industry challenges in the context of EU and international megatrends
5. Identify, define and articulate specific topics that need addressing for integrating existing materials models with experimental data and business criteria
6. Formulate approaches for addressing the indentified challenges and ways for implementation
7. Document the general industry feedback, topical interests and implementation approaches for delivering input for future funding programmes (e.g.in the context of Horizon 2020.)

Desired outcome:

The critical outcome of the team effort is the completion of Road Map for encouraging integration of materials modeling into business decision making delivering a direct impact on the competitiveness of the EU industry base. Eventually the start of bottom-up activities if necessary.

Timeline:

Completion of a Road Map by end Q1 2015

Continuously: Expanding database to reach a representative social network with active core (the team)

Sept 2014: Input to the request for sharing of ideas sent by EC. This request will be sent to the existing list of companies and will have this Charter as attachment

Sept 2014: First draft Road Map as discussion paper for Nov meeting by core team



Oct 2014 Invitation to Nov meeting of active contributors by EC

Nov 2014: Report on outcome of the wide consultation

Dec 2014: Second version Road Map

Team members

Alessandro Curioni – IBM

Massimo Noro – Unilever

Stef van Eindhoven – TU Eindhoven

Peter Klein – Fraunhofer Kaiserslautern

Jean Francois Agassant - Mines ParisTech CEMEF

Iakovos Vittorias– LyondelBasell

Rudy Koopmans – Dow Europe GmbH

Process charts for integrating materials science modeling into business decision making

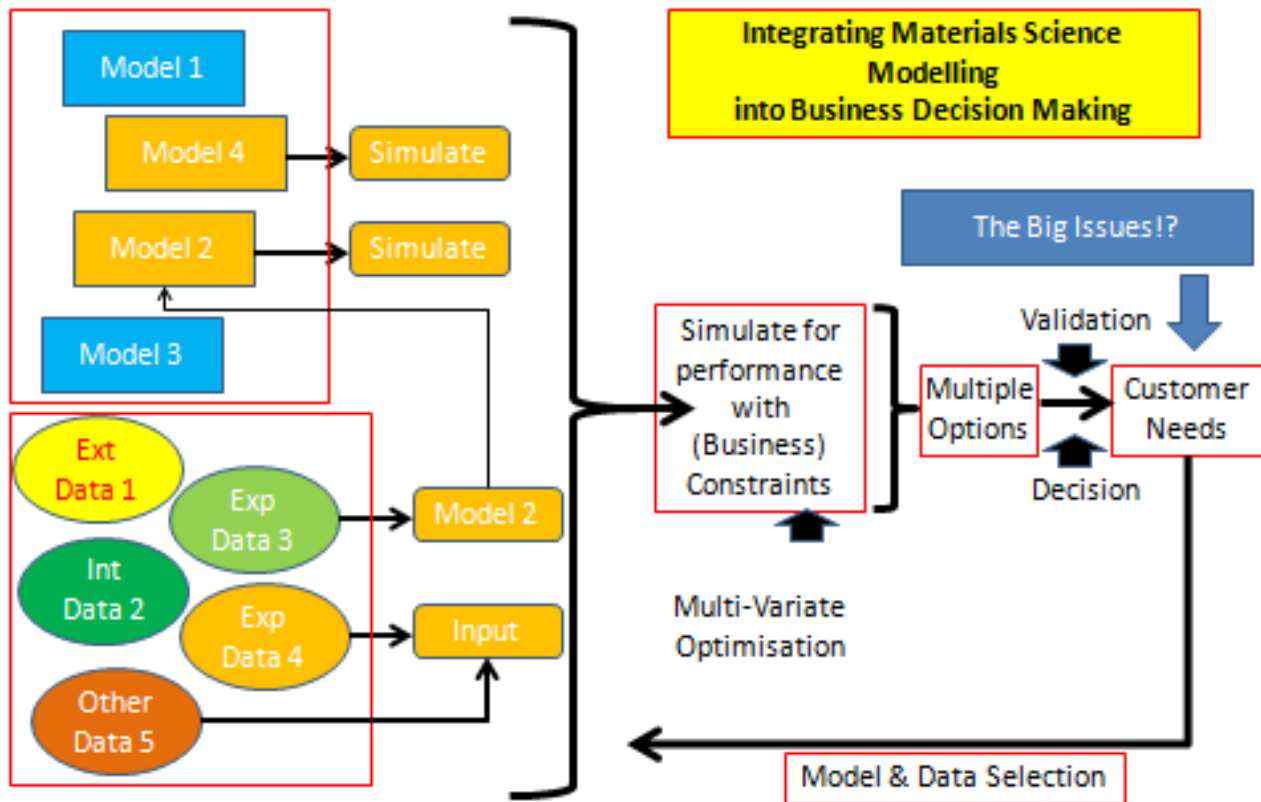


Figure 1: Schematic for integrating of several existing models and data of various sources with business constraints, leading to options for addressing customer needs i.e. product development.

Example Project: Tailored Multilayer Packaging Films

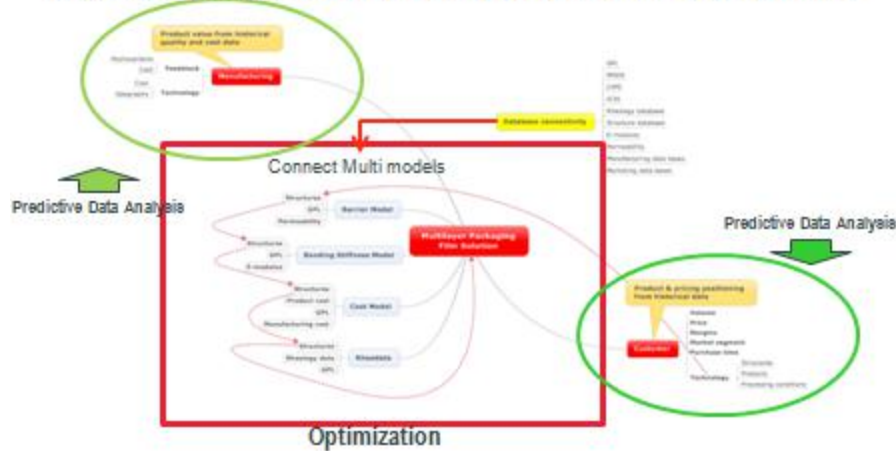


Figure 2: Schematic example for integrating modeling, empirical data, structured and unstructured data with business constraints, leading to options for addressing a multilayer film development for food packaged pouches.

Topics to address:

- Identification of major materials science and technology challenges
- Modularity of models and interconnectivity to flexibly develop modules addressing a technology problem
- Database connectivity
- Integration of simulations with experimental data and commercial constraints
- Multi-variable optimization of multi-model simulations
- ...