EMMC BDSS GUIDELINE 01-2020

Guideline for Business Decision Support Systems (BDSS) for Materials Modelling

European Materials Modelling Council

EMMC BDSS Guideline 01-2020 Joint Working Group

The following is a list of persons forming the Joint Working Group assembled between three European funded projects[1], EMMC-CSA – GA Nº723867, FORCE – GA Nº721027, COMPOSELECTOR – GA Nº721105, and contributors from the respective projects.

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CONTENTS

FIGURES

TABLES

1 INTRODUCTION

Why Materials Modelling?

We enjoy the benefits of materials in almost every aspect of our daily lives, within our engineered world of mobile phones, computers, all modes of transport, processes for energy conversion and distribution, physical dimensions for virtual reality, medicine, our aspirations for quantum computing and space exploration, and at the interface with the natural world such as renewable resources for fuels and energy harvesting, biodegradable feedstocks for manufacturing and low carbon construction. As such, materials are an essential part of our response to societal challenges of health, food security, sustainable use of our natural resources, clean and efficient energy, smart and green transport, creation of a circular economy, and ongoing innovation leadership.

The selection of materials and manufacturing processes for design applications requires knowledge of their inherent properties (strength, density, conductivity, etc.), their states of matter (liquid, solid, gas, plasma) and transitions between states, their performance under geometrical and loading of force constraints, and their in-service performance (temperature, fluid resistance, cyclical loading, etc.). This information is typically based on experimental tests, often using standard representations of the in-service environment. Today, physics-based modelling is proving to be both a challenging and cooperative solution to physical testing by predicting material properties and providing new insights to their mechanisms and behaviour.

Materials modelling is approximating the laws of physics and chemistry that describe materials and related conversion processes such as formulation and manufacturing, or photosynthesis and decomposition in the natural world. These approximations are expressed in mathematical equations. Multiscale modelling is an approach that enables the design of products and the materials which comprise them by linking materials models applied to multiple length scales.

Due to achievements in the accuracy and predictive capabilities of simulation tools (in combination with developments in experimentation), businesses are reporting advances in innovation, revenue generation, faster times-to-market, costs savings and improved understanding. An average return on investment (ROI) of 8 has been reported by manufacturing organisations investing in materials modelling, contributing to benefits such as innovation, cost savings, job creation, and increased revenue [1]. Staff costs, or expertise, is the largest cost factor associated with materials modelling: the ratio of staff/software/hardware costs is reported as 100/20/6, respectively.

In order to embed materials modelling more strategically within organisations and affect higher level processes in the business, there is a need for a Business Decision Support System (BDSS) enhanced by materials modelling [2, 3]. The BDSS should also account for the associated risks, uncertainties and costs related to the modelling and simulation tools and activities. This is a priority especially for small-to-medium enterprises, SMEs, which often require an earlier indication of return on investment compared to large enterprises, LEs. Resulting from the increased information and improved integration with business processes, the BDSS should thus also reduce the costs and risks associated with the adoption of materials modelling.

The 'sweet spots' for the combination of materials modelling and business modelling were identified by manufacturing organisations as [4]:

a) addressing open research questions
b) characterising a material system
c) understanding effects of processing on properties
d) screening hypothetical new materials
e) enabling computer-aided design
f) facilitating substitution (e.g. due to REACH legislation)
g) understanding failure mechanisms

As an exemplar 'sweet spot', we will consider the screening of two typical material properties used in design, strength and density. Screening across 4,000+ commercially available materials, we will find that there are holes or gaps in the property space which have yet to be filled by real materials (Figure 1). Materials filling the first 'hole' in the materials property space (top, left-hand corner) would enable lighter-stronger/stiffer applications as desirable for most transport applications to improve fuel economy, and the second 'hole' is between light-weight honeycombs structures (often made from resin-infused-paper or aluminium to create a stiff structure in compression) and damping properties of elastomers (e.g. properties for 3D printed elastomers could be placed in this hole). If we consider developing a new metal to fill the top, left-hand corner, finding new metal alloys using combinations of the 61 commercially available metals (a subset of the 87 known metals in the periodic table), this approach leads to ~1800 binary alloy combinations, ~36000 ternary alloy combinations, and millions of 'higher order' alloys. Full characterization by testing takes 5-6 years for a new ternary alloy (i.e. to create a phase diagram), requiring upwards of 3000 physical tests (e.g. aerospace qualification, biomedical certification), including testing its integration with other materials in sub/full systems and the in-service conditions. Screening using electronic quantum mechanics modelling and high-throughput development has been proven to reduce this time-to-discovery/identification to 5-10 alloys per day [5].

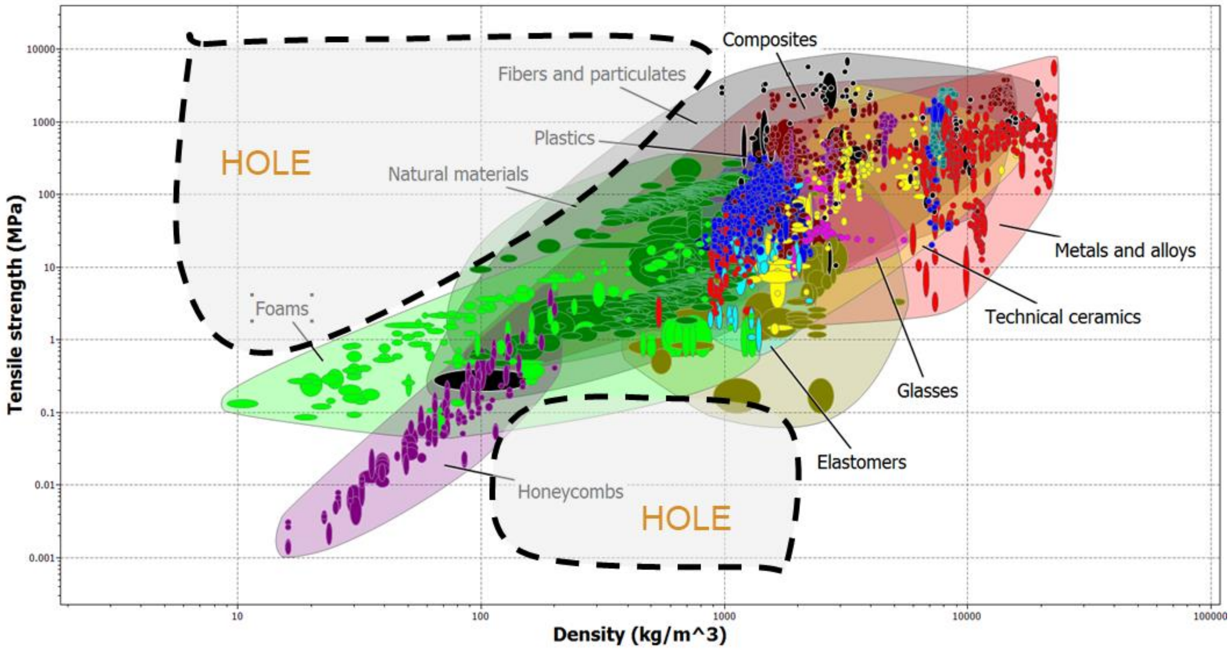


Figure 1: 4,000 commercially available materials plotted against two typical material properties used in design (courtesy Granta Design Ltd.)

Why is a Business Decision Support System (BDSS) needed?

Methods and tools are constantly sought by manufacturing organisations to help reduce the time to reach decisions and solve problems, to reduce the costs of running the business, and to improve solution flexibility by providing different perspectives to a given question or problem. Materials modelling is seen as part of an emerging toolkit to help reach these business goals, however, realising the benefits of materials modelling in development areas such as the 'sweet spots' requires investment in a framework to help materials modelling *plug-in* to the business. Specifically, the following **BDSS 'components'** need attention, and will be elaborated in Chapter 3:

i) a decision-making strategy allowing simulation outcomes to support business decisions
ii) expertise
iii) computational tools (models and simulation codes)
iv) experimental data or their generation
v) digital infrastructure for data management
vi) traceability of decisions
vii) a strategy for quality assurance of the decisions taken

The BDSS concept, or Business-DSS, for integration of materials modelling in business decision-making aims to bring together these seven points by developing a methodology that can support democratisation of materials modelling across industry sectors. A diverse group of stakeholders (end-users) can benefit from the BDSS such as materials and process developers, designers, managers across various business entities, all of which concurrently contribute to business decisions based on design principles and market needs/opportunities. The six points are already integrated (with varying degrees of maturity) for continuum modelling and simulation for example in stage-gate development processes, but discrete modelling is currently not well integrated to the existing infrastructure, and if so, it is only used by large enterprises. Therefore, a need exists to provide a decision infrastructure including the wider scope of materials modelling.

This document describes how the BDSS can help to advance the adoption of materials modelling by manufacturing organisations for decisions on materials and product design and development. Chapter 2 contains general terminology for the BDSS concept and for the discussion of materials modelling and simulation. Chapter 3 outlines the BDSS context related to expert roles or personas related to a working BDSS, methodology related to model selection starting from the business case, etc. Chapter 4 presents an overview of BDSS implementation strategies by the EU projects FORCE and COMPOSELECTOR.

2 TERMINOLOGY

Unless otherwise stated, the terms and definitions for the description of the BDSS concept in this report have been derived by members of the EMMC. Attributes for Modelling and Simulation reflecting the goals of the business (economic and resource efficiency, reduced lead time, verifiable and correct solutions to problems) need to be defined, as they reflect the core function of the BDSS to connect materials modelling and simulation activities and outcomes to business decisions

We will first discuss general terminology and then elaborate these for the BDSS tool itself and for its content. The content consists of Business Entity related aspects and Modelling and Simulation aspects.

2.1 General terminology

Business is the complete (cross-functional) operations of a company.

Business Entity is the business-related object.

Decision Maker is a business entity taking decisions and using the BDSS. Normally the Decision Maker is a person, but in some special cases, the Decision Maker may be an algorithm itself i.e., a software module (like in a self-driving car, or a fuzzy-logic system, etc.) that uses the BDSS tool to make decisions (automatic decision making. The BDSS supports the Decision Maker; The Decision Maker is outside the BDSS; Decisions can be related to optimisation).

Attribute is a quality or feature of the object under consideration.

Attribute Classes are combining attributes.

Performance is the capability (state or level) of an object. The meaning of performance in the context of BDSS is not "execution of a task or function".

Value is an element from an ordered set used to signify the position of an element with respect to other elements in the set, e.g., as a number and unit on a scale of temperature (scale is the ordered set), the colour on colour scales, the string high or low, etc. Ordered sets can contain other ordered sets representing values of higher dimensionality (e.g. tensors).

Target is a goal or objective and in the context of this paper it can relate to 1) feasibility decision (threshold values, yes/no), 2) performance decision (e.g. specific value, or range of values). The Target is set in the context of BDSS by the decision maker or by a minimisation/maximisation (optimisation) process.

Indicator is the expression of the state or level of the relevant Attributes.

Performance Indicator (PI) is an indicator that expresses the state or level of the relevant Attribute. The PI itself is not the outcome of the process on judging the performance, but rather the PI can be used in the judging process. The judging is done by the decision maker and is based on target values of the performance indicator (see Key Performance Indicator).

Key Performance Indicator (KPI) is a performance indicator that has a target value and is declared to be of importance to the company. A KPI can be a combination of one or more performance indicators, e.g. in objective functions. A performance indicator can be declared to be a key performance indicator if there is a target value related to it.

KPI Value is a value of the KPI.

Acceptance Criteria is a terminal (maximal, minimal, nominal, specific, etc.) value or range of key performance indicator values that can be accepted (and set) by the decision maker. KPI's are used in tandem with Acceptance Criteria to assist and support decision making; by comparing the KPI Value to the Acceptance Criteria values a decision can be reached. For example, temperature in a specific range indicate maximal engine power (the performance).

ROI is the return on investment and is defined as the ratio of Benefit-to-Cost for material modelling activities. An assessment/calculation could be validated against various levels of performance within a manufacturing organisation: individual projects or applications, departments, individual sites, across the organisation, and/or across the supply chain.

NPV is the net present value of a product incoming cash flow over time, $NPV = R_t / (1 + i)^t$, where t = time of the case flow, i = discount rate, and R_t = net cash flow.

2.2 Terminology related to the BDSS-tool

In this section we discuss (using the above defined concepts) what a BDSS is and what the attributes are companies require from this tool.

A **Business Decision Support System** (BDSS) is a system (most often implemented in a software tool) that supports an organisation to take informed decisions across different operations of the company:

- Two main elements of a BDSS are 1) flow of information, and 2) interaction of information.
- A BDSS collects, generates and assimilates data from different sources (internal and external) for effective and informed business decision making.
- Key Performance Indicators (KPIs) are used to compare actual values of chosen Attributes with Target Values. Note that KPIs for content aspects in the BDSS tool are evaluated by the BDSS system using e.g., modelling workflows, databases, cost sheets.

- The BDSS combines sources of information, possibly including results of simulations, to calculate values of the Attributes.
- The BDSS provides support for the decisions to be taken by a decision-maker and can do so in the form of optimising across KPIs.
- For many business operations, management software exists (like Product Life-Cycle Management, PLM for managing the product or Enterprise Resource Planning, ERP for managing resources) and these become a source of information for the BDSS
- Business operations can include life cycle management, product management, human resource management and enterprise resource management.

Attribute Classes for the BDSS tool(s) describe the end-user and tool provider perspectives, as detailed in Table 1. The presented grouping of attributes into classes (classification) was supported by a BDSS Expert Meeting held in March 2018, Brussels. The Meeting Report [4] provides several examples (167) of Tool Acceptance Criteria against these classes.

Table 1: BDSS-tool Attribute Classes for simulation, and example Attributes and Descriptions

BDSS Attribute Class	Attribute	Attribute Description
Economics of simulation	Cost, Time, ROI, NPV, …	Cost and time related to infrastructure, personnel to implement and maintain the BDSS, software licences, high performance computing if necessary (HPC), etc. ROI and NPV are methods to express monetary benefits.
User Experience On simulation tool	Ease of Use, …	Functional requirements of stakeholders for ease of use of models/simulation tools/data/information/outcomes, familiarity.
Value Proposition For using simulation	Quality, Benefits, …	In marketing, statements regarding industry challenges and the value of a solution to customers. Statements are qualitative and quantitative (notably addressing economic value). Solutions may be products or services.
Technology (simulation software and hardware)	Maintainability, Interoperability, Reusability, …	Non-functional expectations of technology to ensure aspects such as security, interoperability, traceability, etc.

In the coming two sections we discuss the content of a BDSS. First, we discuss the business part to be incorporated in the BDSS tool and thereafter in 2.4 we discuss how simulation tools could be incorporated.

2.3 Terminology related to Business Entities that play a role in the BDSS-tool

Table 2 provides an outline of Business Entities (or typical departments) which influence and/or take business decisions. Generic attributes to describe performance and/or decisions and design phase selection requirements are associated in this table with business entities to provide context for the materials, process, product decisions which might be associated with the BDSS. Performance of the Business Entity might not have a target/objective; while in other contexts, performance means how close the Business Entity is to its objective, or how successful it is.

Table 2: Business Entities and associated attribute examples

Business Entity	Business Entity Attribute
Finance/Procurement	Return on Investment
IP Management/Legal	Freedom to Operate
Regulations	Risk Assessment
Marketing	Business Strategy
	Market Opportunity
	Market Readiness
Supply Chain Management	Customer
	Supplier
Human Resources	Skills Investment
	Resource Management
Health, Safety, Environment	Sustainability
	Safety
	Risk
Information Technologies	Security
	Reliability
Product Development	Materials
	Manufacturing Process
	Structural
	Product Design
	Modelling & Simulation
	Life cycle assessment
	Resources (supply, technology, consumables)

2.4 Terminology related to Modelling and Simulation used in the BDSS-tool

Modelling and simulation activities related to material design, product design and manufacturing require definitions for aspects of verification, validation and uncertainty quantification (VVUQ). This section reports common terminology accepted by industrial end-users and has been referenced from open documentation.

Given the focus of BDSS on materials modelling integration, we will list definitions based on the ROMM (Review of Materials Modelling, [7]) and its standardisation as agreed in CEN Workshop Agreement (CWA) 17284 [8] (formalized definitions based on the ROMM). This taxonomy was established to harmonise the languages of the four modelling communities: electronic, atomistic, mesoscopic and continuum. As the BDSS will be used by materials and product design experts, modelling and simulation terminology used in continuum communities (in particular NAFEMS and ASME) is briefly reviewed and contrasted in the hope the presentation makes the BDSS easily accessible for both materials and product design experts. The other three modelling communities also have their vocabularies like e.g. atomistic modelling, but an exhaustive review is beyond the scope of this document.

Here we briefly recap some general terms related to modelling used in many sectors, but which are largely independent of the domain of use.

Physical Model is a smaller or larger physical copy of an object [9].

Conceptual Model is a representation of a system, made of the composition of concepts which are used to help people know, understand, or simulate a subject the model represents. More specifically in materials and engineering modelling it refers to the collection of assumptions and descriptions of physical processes representing the behaviour of the reality of interest from which the mathematical model and validation experiments can be constructed [10].

Mathematical Model is a description of a system using mathematical concepts and language [11].

> Note: The term Model is also used to refer to the geometrical and computational representation of materials or the product. For example, ‘a molecular model’ may refer to an actual physical ‘ball-and-stick’ model of a molecule or a mathematical model of the same, or a computational representation of how atoms form a molecule.

> Note: The ASME and NAFEMS definition of Conceptual Model and Mathematical Model include boundary values and initial conditions required for a simulation [10].

Numerical code or software or computer code is the computer implementation of algorithms developed to facilitate the formulation and approximate solution of a class of problems [7, 8, 10].

2.4.1 Terminology related to Materials Modelling and Simulation

If we now concentrate on materials, we follow the RoMM [7] and CWA 17284 [8], and the materials modelling and simulation terminology is defined as follows.

Computational materials models are understood to be physics-based models, i.e. data-based models do not form part of the definitions.

A **Physics-based model** is a solvable set of one Physics Equation (PE) and one or more Materials Relations (MR). The **Physics Equation (**PE) approximates a physics law. The **Materials Relations** (MR) describe a specific behaviour, providing values for the parameters in the PE. Together, PE and MRs form the **Governing Equations** [7]. Neither the PE nor MR can be solved in isolation, but it is the application of the PE to a specific case 'documented' by the Materials Relation(s) which can be solved. MRs include the constitutive equations used in continuum models as well as the Hamiltonian in electronic models and the force fields in atomistic models.

> Note: In continuum mechanics, the Materials Relation (the Constitutive Equation) are often referred to as the "Material Model". That is understandable in the context of a field dealing with a single (conservation equation for continuum mechanics or fluid) PE which thus does not need to be mentioned, and where modelling (i.e. exploration of the Governing Equations) is largely concerned with the Materials Relations, which then are often referenced by a *totum pro parte* "Material Model" [12].
>
> Likewise, the atomistic Molecular Dynamics community is using only one PE (Newton's Law) that does not change, and the field is concerned with modelling the Materials Relations called force fields (interatomic potentials). They also often refer to their MR as 'models'; and this can again be explained as within that community this is the part of the governing equations which the end-user varies.
>
> The RoMM with its objective to give all parts a separate name has not adopted such merged notions and has thus restricted the meaning of the word model.

Constitutive Equation, or constitutive relation, in physics and engineering is a relation between two (or more) physical quantities that is specific to a material or substance and approximates the response of that material to external stimuli, usually applied fields or forces [13].

Simulation is the complete set of activities to arrive at a calculated answer to a specific question, particularly the execution of the model on a User Case using a solver and postprocessor. This is done via (numerical or software) code(s) [7].

> Note: ASME shares a similar definition wherein Simulation is the computer calculations performed with the Computational Model [10].

Solver is a numerical method used to solve the Physics Equation complemented by the Materials Relations applied to a User Case with its boundary values and initial conditions [7].

> Note: In the continuum world, the term Solver and the terms code and Computational Model are all used for the numerical implementation of the mathematical model, usually in the form of numerical discretisation, solution algorithm, and convergence criteria [10]. The RoMM with its objective to give all parts a separate name has not adopted these merged notions.

Pre-processing is an operation (or set of operations) to prepare input data for a simulation, such as calibration of model parameters using experimental or simulated input values from a database [7,8].

Post-processor is an operation (or set of operations) on the data set resulting from the solution of the PE+MR applied to a User Case done in order to extract useful information, such as homogenisation of material properties, or visualisation of results [7,8].

Simulation Results are the output generated by the computation model [10], or Solver and Post-Processor [7].

Simulation Outcome refers to features of interest extracted from Simulation Results that are further processed for example by statistical analysis and/or uncertainty quantification. Simulation Outcomes, along with estimates of the uncertainty, can be used for comparison with experimental results for validation [10].

Calibration is the process of adjusting physical modelling parameters in the computation model to improve agreement with experimental data [10]. The same concept is used in ROMM documentation as applied to Materials Relations (MR) [7].

Prediction is the Result, Outcome from a simulation that calculates the behaviour of a physical system before experimental data are available to the user. Predictions come with errors and uncertainties because of limitations in numerical accuracy, approximations and deficiencies in the model, uncertain initial and boundary conditions, and uncertainties in the system and/or the environment [14]. A range of Simulation Outcomes that represents real-world variation in behaviour is a valid prediction.

2.4.2 Terminology related to Verification, Validation, Uncertainty Quantification processes

Verification (adapted from [10, 14, 15]; also described in [16]) is the process of determining that a model, solver and post processor-implementation (numerical code) accurately represents the developer's conceptual description of the model and the solution to the model. Verification is a coding task that deals with the estimation of all relevant sources of numerical solution error in an actual application model, which include: i) computer round-off error; ii) iterative solution error; iii) discretisation error in space, time and frequency; iv) statistical sampling error; and, v) response surface error. If the estimate of each error is not feasible, then the sensitivity of the simulation results to these should at least be investigated. This definition is sometimes termed **Calculation Verification** and its accuracy is sought quantitatively, and **Code Verification** refers to whether or not the computer code is correct and functioning as intended and is an assurance practice that aims to remove all errors in the code. Verification is a software producer's responsibility, and as many manufacturing organisations develop their own in-house codes, they also execute this task. Modern Software Quality Assurance techniques exist and are applied to testing of each released version of the software. Sometimes the users can develop their own post processors and then the users of software share in the responsibility for code verification.

Validation (adapted from [10, 14, 15, 17]) is defined as the process of determining the degree to which a model (approximation of the physics, PE + MR, for a materials model) is an accurate representation of the behaviour of a physical model (i.e. real world sample or specimen) from the perspective of the intended uses of the model. Validation included the assessment of the error due to the approximations and assumptions made in the formulation of the conceptual model, the physics equation and the materials relations. We will also include the validation of all aspects that describe the User Case and the physics-based approximations in pre/post processing steps, representation of boundary conditions, material structure, and simulation inputs such as properties, etc.

The assessment of error is achieved by comparing simulation results against Reference Values. We have to be aware that these last may in themselves have errors as experimental data drawing on specially designed and executed experiments for a hierarchy of physics and system complexity have several potential points of error from equipment calibration, data acquisition rates, environmental control, complexity across scales, etc.

Validation is a task typically done: 1) by the modeller/code owner when developing the model that is to be coded up to determine its applicability domain; and, 2) by the end-user to ensure the User Case at hand is well represented by the physics approximations.

For advanced users who are also code developers Verification and Validation are an iterative and "coupled" process, wherein all aspects of a simulation (including the Model, Reference Values, Code, solver calculations), are evaluated for uncertainty (see Uncertainty Quantification). The order in which sources of errors/uncertainties (e.g. validity of User Case information, models, experimental tests and veracity of codes, calculations, etc.) are evaluated depends on their influence on simulation outcomes (or from the perspective of the industry end-user, their influence on design and safety). An iterative approach is illustrated in ASME and NAFEMS documents (specifically, see Figure 4 of reference [10]).

Reference is data, theory, or information against which simulation results will be compared [10].

Validation Experiments are designed and performed to generate data for the purpose of model validation [10], and to assess the accuracy of a simulation prediction on a certain User Case [7]. A validation test will explore the variation in the physical model, i.e. specimen geometry, initial conditions, boundary conditions, and all other parameters (of the User Case) [10, 13, 14, 15]. The material structure and/or material behaviour of the physical model (test specimen) must be measured with the highest possible, quantified accuracy [7].

Validation Metric is a mathematical measure that quantifies the level of agreement between simulation outcomes and experimental outcomes [10]. Validation Metrics are established during the development of the conceptual model and may be reported as percent difference, or a range (+/-), such as [17]:

- The expected value of the error, E(e), or the variance of the error, V(e), if the error, e, between experimental data, y, and model prediction, y* , is given by e = y − y* , a simple metric could be
- P(e > 0) , where P(·) is the probability; the 95th percentiles on the probability distribution of e ; or a hypothesis test such as E(e > 0), where the validation metric is a pass/fail decision of whether or not the model is contradicted by the data.

Verification Metrics are typically defined as errors as done for Validation metrics. There is no formal definition for Verification Metrics, but the intent is to mirror the quantitative reporting requirements of Validation Metrics. They may be quantitative measures and are often statistically based.

Uncertainty Quantification (UQ) is the process of characterising all uncertainties in the model or experiment and of quantifying their effect on the simulation or experimental outcomes [10]. There are established methods (e.g. nondeterministic methods) for UQ.

Experiment is the observation and measurement of an experimental system (physical model) to improve fundamental understanding of physical behaviour, improve physics (and then mathematical) models, estimate values of model parameters, and assess component or system performance [16].

Experimental Data is the raw or processed observations (measurements) obtained from performing an experiment [10]. Uncertainty in the measured quantities should be estimated so that the predictions from the simulation can be credibly assessed [15]:

- Uncertainty and error in experimental data include variability in test fixtures, installations, environmental conditions, and measurements.
- Sources of nondeterminism in as-built systems and structures include design tolerances, fluctuations in the environment (weather) or power supply (electricity),

residual stresses imposed during processing, and (not-characterized) variations of materials from batch production.

- In experimental work, errors are usually classified as being either random error (precision) or systematic error (bias).
    - An error is classified as random if it contributes to the scatter of the data in repeat experiments at the same facility. Random errors are inherent to the experiment, produce nondeterministic effects, and cannot be reduced with additional testing.
    - Systematic errors produce reproducible or deterministic bias that can be reduced, although it is difficult in most situations. Sources of systematic error include transducer calibration error, data acquisition error, data reduction error, and test technique error.

Experimental Outcomes are features of interest extracted from experimental data that will be used, along with estimates of the uncertainty, for validation comparisons [10].

VVUQ is an acronym for verification, validation and uncertainty quantification [15]. The expected outcome of the simulation VVUQ process is the quantified level of agreement between experimental data and simulation prediction, as well as the predictive accuracy of the model. A key component of the integration of simulation VVUQ into the quality-assurance process is the documentation of all relevant activities, assessments of VVUQ program adequacy and completeness, and peer reviews at various stages of the program.

2.4.3 Example attributes and classes for Modelling and Simulation used in the BDSS

The table below summarises attributes used to describe modelling and simulation. Special attention is given to VVUQ as these influence the decisions surrounding the use of modelling and simulation activities in a business. But the KPI related to business entities will not be forgotten, e.g. Economic, Management classes. This example uses specific attribute definitions and they are given after the table. This list of attributes is not meant to be exhaustive but does represent the types of attributes used in BDSS projects FORCE and COMPOSELECTOR funded by the European Commission. The attributes are grouped in classes.

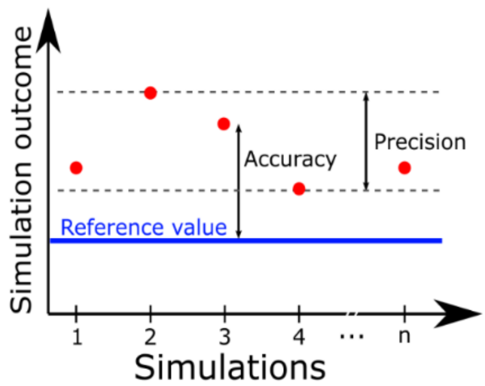
Table 3: Example attributes and their classes and their descriptions related to modelling and simulation tools

Modelling, Simulation Attribute Class	Attribute (Examples)	Attribute Description (Examples)
Economic	Time, Cost	Time and Cost of expertise, software license, HPC, for specific modelling/simulation workflows.
Management	Completeness	Qualitative assurance measures embedded in governance processes. These can include peer review, experience and expertise of personnel and the organisation, and maturity in performing certain classes of simulation.
Verification (Calculation)	Sensitivity, Confidence, Uncertainty	Quantitative measures, often statistically based, to estimate the numerical error in the quantities of interest. Calculation verification is required to quantify the numerical accuracy of the uncertainty analysis [15].
Verification (Code)	Confidence, Error, Margin of Error, Uncertainty	Quantitative measures to define the correctness of the code against benchmark problems; Software Quality Assurance is part of the verification process [10].
Validation (Model)	Accuracy, Precision, Reliability, Confidence	Quantifiable measures, often statistically based, to describe the Accuracy and Precision of a material model (PE and MR) outcome against an experiment, and may be defined by a Validation Metric; the term Reliability may be used to express the generic nature of the physics approximations that is the consistency of validation results over a range of User Cases including boundary conditions and/or repetitive use of the model by multiple users; Uncertainty Quantification may be used when the variability of multiple inputs to model parameters can be considered. See also Validation Metric.
Validation (Simulation)	Accuracy, Precision, Convergence or Stability,	Quantitative measures to evaluate simulation outcomes on a particular User Case against physical tests in terms

	Robustness, Confidence, Convergence, Uncertainty	of Accuracy and Precision, often leading to further Calibration activities. Simulation outcomes Convergence or Stability (e.g. mesh size, number of molecules or atoms) to reach a target level of accuracy; Robustness refers to the consistency of Accuracy and Precision over a range of boundary conditions, the consistency of results (or rate of failure of results to reach targets) which may be defined as Reliability; Uncertainty Quantification may be used when the variability of multiple inputs from experimental or simulation sources must be considered in the final simulation outcome.

The description of the attributes mentioned in the above table are as follows:

Accuracy is the closeness between the result of a measurement and a “true value” of the subject being measured; it is historically a qualitative measure indicating a high/low relationship to a ‘true’ value, but is readily used as a quantitative measure with an associated ‘+/-‘ value (although this is not in agreement with the first definition).



Precision is the closeness of the measurements to each other. It may also refer to the refinement in a measurement, calculation, or specification, especially as represented by the number of digits given.

Fidelity is a term often used to indicate the difference between simulation and experimental outcomes [15]. See also Validation Metric.

Error is a recognisable deficiency in any phase or activity of modelling and simulation that is not due to lack of knowledge [10].

Margin of Error refers to the accuracy of the model/simulation expressed in percent. (see ROMM [7]).

Uncertainty is a potential deficiency in any phase or activity of the modelling, simulation or experimentation process that is due to inherent variability (irreducible uncertainty) or lack of knowledge (reducible uncertainty) [10, 15]. Irreducible Uncertainty is the inherent variation associated with the experimental system being modelled; Reducible Uncertainty of the models is the potential deficiency that is due to lack of knowledge, e.g., incomplete information, poor understanding of physical process, imprecisely defined or nonspecific description of failure modes, etc. [15].

Convergence (Stability) is the successive refinement of model or simulation parameters, e.g. mesh, time step, size of simulation box etc., until a target level of accuracy is obtained. Parameters in this context refer to quantities from which the results of the simulation should be independent. Convergence may be measured in terms of Accuracy and Precision.

Reliability is a measure of the *probability of failure* on a specific User Case due to inaccuracies in the code and/or model (against an analytical or benchmark solution), or simulation results not meeting targets for Accuracy and Precision as defined by validation experiments. Reliability statements are often combined with statements about risk [7, 14, 15, 18]. For a modelling/simulation User Case of a system comprised of multiple components, Reliability of the system may be based on [19]: 1) assessing the probability of each possible component failure state; 2) determining the system behaviour resulting from each component failure state; and 3) combining the first two components to obtain an overall probabilistic index of system reliability. Reliability is often coupled with statements of risk to the business. Reliability-based optimization presents uncertainties as constraints with quantified probabilities [19].

Robustness is the *degree of Sensitivity* of performance (e.g. code, model, simulation results) to deviations from normal boundary conditions. Unlike the three ways of assessing reliability, assessing robustness generally consists only of determining the system behaviour resulting from each possible component failure state (point 2 of Reliability); that is, there is no assessment of the probability of a given component failure state occurring. Robust design optimisation aims to find a solution as insensitive as possible to uncertainties. Robustness of materials data to User Case conditions is another application of the term [18, 19].

Complexity may refer to the number of tiers in a hierarchy of physical relationships, for modelling or experimental purposes, and is important for V&V activities [15]. The Figure below shows a schematic of a generic hierarchy, with tiers representing the complete system, subsystems, components and unit problems; the number of tiers needed to deconstruct a system into a series of fundamental physical problems. Complexity, or Simplicity, is not necessarily a reflection of Accuracy and Precision, but may be related to economic attributes such as Time and Cost (e.g. multiple software licences, time to convergence, experimental validation). The system and subsystem tiers typically represent physical assemblies. Examples of unit problems include material coupon tests, interface or joint, and load environments. Component problems typically involve simplifications of idealized geometry and simplified boundary conditions, etc.

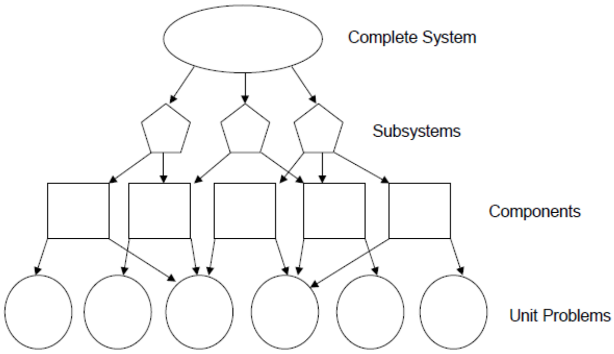


Figure 2: Example hierarchy of system complexity [15]

Sensitivity analysis is a formal process for identifying which underlying uncertainties contribute the most to uncertainty in key simulation results [14] and/or in KPI Values. Sensitivity analysis is invaluable in focusing on subsequent simulation or experimental efforts; should management decide that uncertainties need to be reduced or better decisions need to be made to reduce risk (e.g. the sensitivity of model parameters helps the end-user understand the most-to-least influencing parameters on the simulation outcomes).

Confidence is the probability that a numerical estimate or experimental test result will lie within a specified range.

Completeness is the qualitative measure embedded in governance processes for VVUQ best practices and including peer review, experience and expertise of personnel and the organisation, and maturity in performing certain classes of simulation.

3 BDSS CONTEXT

The seven components of the BDSS methodology outlined in the INTRODUCTION can be described at a high-operational level as follows and more detail on the first two components will follow in subchapters.

i) **a decision-making strategy using modelling outcomes to support business decisions:** the BDSS supports an organisation to take decisions for development/maintenance of a product and/or production process. Information transactions and decisions are connected by a 'decision-making workflow' which combines individual actions for information requests, information input, decision-making, and decision authorization for a specific decision-making process. Product and/or manufacturing process decisions are driven by KPIs (Key Performance Indicators), their targets and respective acceptance criteria or constraints. KPIs may be business (financial, marketing, regulations, resource availability, etc.) and/or technical (material or product properties, manufacturability, etc.), or a combination of the two.

ii) **expertise:** the BDSS end-users are divided into three high-level personas - Business Manager, Senior Manager, and Operations Personnel.
iii) **computational codes:** the ROMM [7] provides a classification of models developed to support materials modelling. Marketwise, the majority of discrete materials modelling codes is developed and maintained by SME [20] and it is well established that there are many codes reaching a high quality within academia/research as evidenced in the ROMM [7]. Continuum codes are already well-established in the market.
iv) **experimental test data or its generation:** sources of information may include experimental characterization, primary data measurements from equipment/sensors, customer feedback of in-service performance, etc. Experimental data is important for verification and validation of modelling and simulation outcomes.
v) **digital infrastructure for data management:** the BDSS aims to be *interoperable* by making the language (taxonomy, as outlined in the RoMM [7] and EMMO [21]), for simulation activities consistent and thus making information and data exchange accessible for end-users. Data management is required for both experimental and simulation workflow.
vi) **traceability of decisions:** the overarching BDSS strategy incorporates stakeholders and their decision-making workflows for life cycle management (product/process development and management), human resources management, and enterprise resource management (sustainability, societal and regulation requirements). Digitalisation of the decision-making workflow enables a degree of automation of the various information transactions and decision-making actions, including execution of simulation codes and/or test programs and retrieval of outcomes, analysis and evaluation of information. Traceability is an important topic for industries required to report to regulatory authorities.
vii) **quality assurance:** for a materials simulation outcome to be useful, it must be trusted. Governance of materials modelling and simulation outcomes are an important role within the expertise of BDSS end-users. The EMMC has created quality assurance guidelines that respond to this purpose [22, 23, 24], and NAFEMS also has a guideline for simulation quality management based on ISO 9001:2015 and NAFEMS ESQMS:01 [25].

3.1 Decision-making Strategy for using Simulation Outcomes with Business Decisions

Creating a decision-making strategy starts with the identification of appropriate business needs or objectives for a given User Case and relating these objectives to KPIs (performance indicators that have a target value and are declared to be of importance to the company). The KPI is made up of Attributes which describe the state of the material, product or manufacturing process, acting as variables which can be tuned to meet the KPI target, or fixed constraints. A level of required accuracy, uncertainty and importance may be placed on the individual Attributes, or on the KPIs themselves when multiple KPIs are assessed. Models are then selected (or a modelling workflow of linked and/or coupled models) which can meet the requirements. For each granularity of the model (model entity) needed for calculating the Attributes (and consequently the KPI) there are a set of Physical Equation, PE (see the four chapters for electronic, atomistic, mesoscopic and continuum model entities in the ROMM [7]). The KPIs related to simulation include both theoretical (PE and MR), practical (computing power, time-to-solution) and other aspects, such as available expertise and resources. The accuracy and reliability of the model is heavily determined by the accuracy of Materials Relations (MR). The MR needs User Case information, which in turn also have an associated accuracy. The figure below shows the sequence of the BDSS translation task from User Case definitions to model selection.

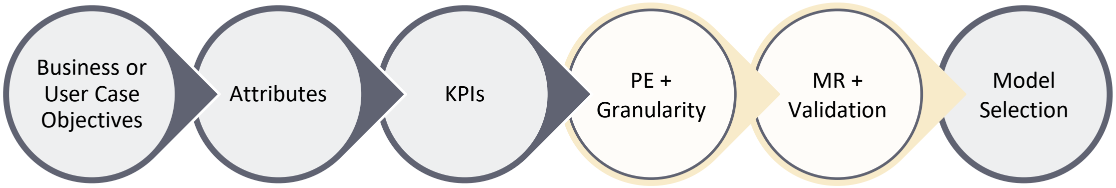


Figure 3: Materials model selection based on Business or User Case objectives

The steps to create a KPI can be outlined as follows:

1. Identify and quantify the true benefit (including success criteria, or target) to the end-user, business, and/or product, when possible

    - Define Quantitative Target(s) – comparable against a benchmark, for example typical targets could include: reduced time-to-market, reduced number of experiments, increased market share, or increased profit, improved resource efficiency, reduced product failures during manufacturing, and in-service, light-weighting, etc.

    - Define Qualitative Target(s) – for example, improved insight and understanding of processing and material, broader awareness of advanced tools and methods, R&D strategy development, etc.

    More business benefits related to materials modelling can be found in Appendix A.

2. Translate the Target into known Attributes

    - Define the target by specifying a value, accuracy, units if quantification, or True/False or ranking for screening if qualitative

    - Identify which Attributes are variables (performance, free), objectives or constraints.

3. Create KPIs related to material, process, part, business performance

- Confirm KPI(s): check their unit, lifetime, target, measurability
- Set the decision criteria: minimize, maximize, TRUE/FALSE
- Decide decision-making process for multiple KPIs: Trade-off (equalise)
- For each Attribute, understand how it can be obtained (available data, modelling), and when it is introduced (design phase), and whether a link to the accuracy of the KPI is required.

3.2 Expertise - BDSS Stakeholders

Three levels of internal stakeholders contribute to the governance of the BDSS, defined at a high-level as the Business Manager, Senior Manager and Tactical Operator. The classification of these levels was supported at the BDSS Expert Meeting [4] and align well with the governance best practices promoted by NAFEMS [14]. The majority of BDSS stakeholders to-date have been representatives from large enterprises, and as such they have the resources to create different types of employees, whereas many smaller-to-medium enterprises have only a handful of persons, or do not have in-house expertise specific for materials modelling, and in these companies all three types of employees might be the same person, or external personnel is to be found.

The **Business Manager** is an individual such as a Vice President (VP) or Director for Product Engineering or Materials and Process entity within the business. In the context of the BDSS terminology, the Business Manager is the Decision-Maker. Their objective is to deliver the product on-time, on-budget, to the requirements of the client, market drivers and regulations. The Business Manager may report directly to the COO/CEO in an SME or to a VP/Director in a larger organisation and has reports from e.g. the Technical Manager as described below. The main tasks of the Business Manager in relation to the BDSS are:

- Maintains an overall perspective on the goals and objectives of the business
- Be responsible for business risks
- Develops the business case or mandate for a product or project
- Establishes the business KPIs (may be technical and/or economic) and their acceptance criteria
- Understands or creates the business workflow between stakeholders for decision-making, ensuring quality criteria of the business are met
- Has business authority for product/project/budget approval
- May, or may not, have modelling experience

The **Senior Manager** has a combined technical and managerial role and is often a materials and/or process scientist or engineer with materials modelling expertise. Their main objective is to deliver materials knowledge and information often in the form of data. The Senior

Manager reports to the Business Manager and creates reports on the operations of modelling/simulation (in smaller organisations, these roles are combined).

- Translates the business KPIs to technical attributes for product, process, model and simulation; may set acceptance criteria, notably for model and simulation attributes
- Creates a decision-making workflow for model selection, a strategy which links model outcomes with business objectives
- Selects/approves input data to the model/simulation process
- Contributes to the design of the validation experiments
- Formulates software tests for code verification, develops procedures for model validation, and provides guidelines for characterising types of uncertainties in an analysis, as well as prepares product design rules for specific application areas [14]
- Reports on the validated business KPIs to the Business Manager

The **Operations personnel** is often a materials and/or process engineer or scientist with materials modelling expertise, but without business decision authority, and may have more experience in modelling compared to the Senior Manager. Their main objective is to deliver validated modelling/simulation outcomes to the Senior Manager.

- Application of guidelines and design rules [14] as set by the Senior Manager, may be in a production simulation environment in a medium or large enterprise (unlikely to have production-scale simulation activities in a small enterprise, unless it is a consulting firm)
- Prepares pre/post processing information/data for modelling/simulation activities
- Prepares the workflow for model selection
- Applies approved input data
- Runs the code or analysis
- Prepares output data and metadata
- Reports on the validated modelling attributes to the Technical Manager

The generalised workflow between the three levels of activities is described in the Figure 4 below. The Business manager executes strategic tasks; the senior manager executes tactical tasks and the operations personnel do the operations. Tactical level tasks, most notably translate the business KPIs to technical attributes for product, process, model and simulation, have been described in the EMMC Translators Guide [26]. Tactical and operational level activities could be performed and/or supported by external experts, such as translators and modellers notably for small enterprises.

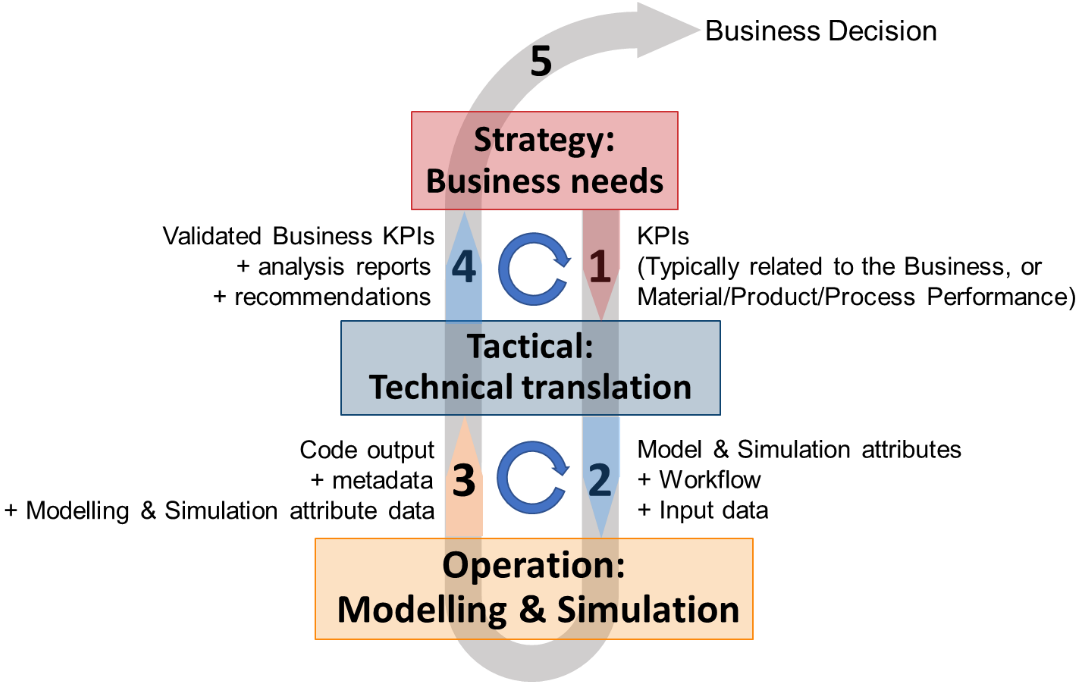


Figure 4: BDSS generic workflow between level of business entities or stakeholders

A further breakdown of the tactical and operations steps of the Senior Manager and Operations Personnel is illustrated in the Figure 5 below using representative icons for each step. The individual steps and related icons are explained below the Figure.

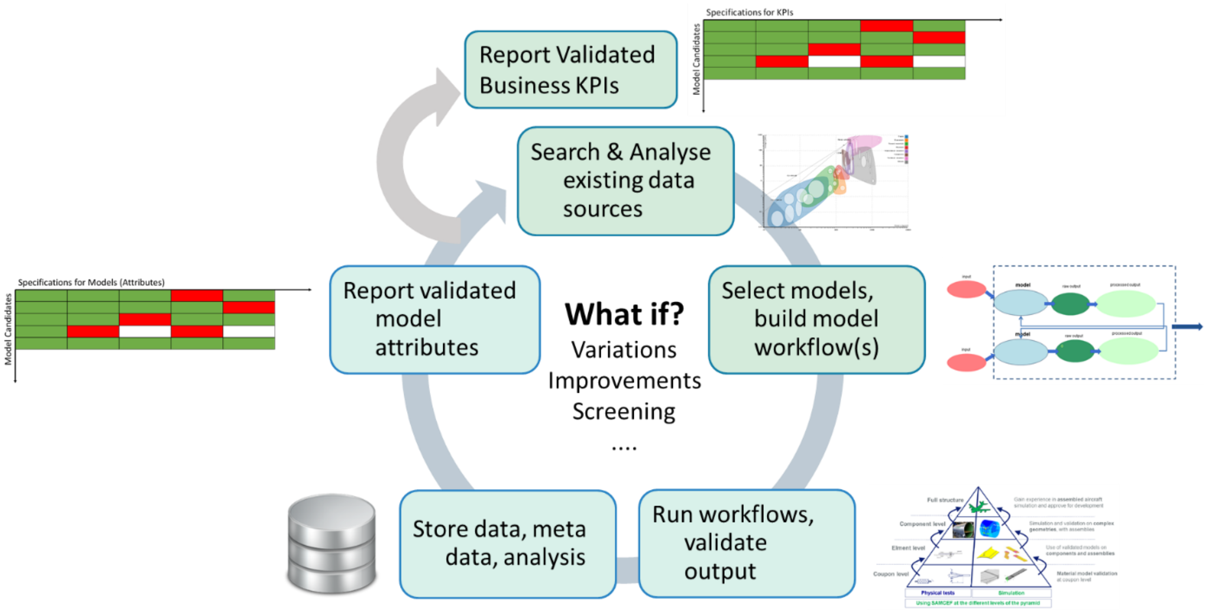


Figure 5: BDSS generic tactical and operation steps

Search and analysis using existing data sources is a first response to the business KPIs specified (value, targets, acceptance criteria) by the Business Manager in the relation to the business case or project/product mandate. The chart to Search & Analyse existing data sources represents a wide range of material property data available to the tactical team, as explained earlier using Figure 2.

When modelling activities are required to fill the gap in knowledge or data, a modelling workflow is constructed to select appropriate models for the application, and to understand their input/output requirements and linking and coupling status. A standard description of a simulation workflow structure was established in the ROMM and in the CWA using specific taxonomy and its documentation is the MODA (Modelling Data) [7]. Below is an illustration of an iteratively coupled workflow using the MODA taxonomy.

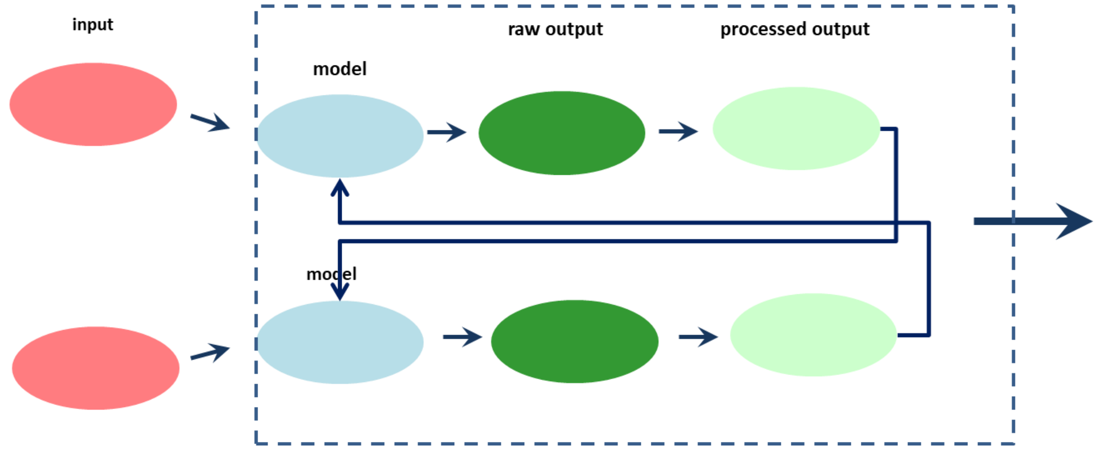


Figure 6: Example MODA for an iterative, materials simulation workflow

Validation of the simulation outcomes using physical experimental outcomes to check the accuracy can be conceptualised for multi-scale modelling (a workflow of models applied to phenomena at different length and time scales) using the building block approach. The building block approach is represented in the pyramid diagram where on one side the physical structure is shown and its complementary model on the other side. The pyramid represents the multi-scale approach to modelling (output of models applied to the lower scale acting as input to models applied to higher or larger scales). The base of the pyramid refers to materials. To decide on materials properties may require 1000's of tests depending on industry regulation. This multi-scale approach is depicted for aerospace part modelling (as illustrated in Figure 7 for aerospace applications) but can conceptually be applied to applications of materials modelling at different levels in many other industrial areas.

Storage of data and metadata is critical to interoperability and to quality assurance of modelling and simulation results, including reproducibility of results. Decision-making based on experimental and simulation outcomes. The decisions must be defensible and based on credible evidence which needs to be readily traceable and have full metadata (or pedigree) for data reviews by peers and regulatory bodies. Business Managers set quality standards as part of their risk management strategies for traceability, and ensure they are followed. Appropriate infrastructure is ensured for the management and security of data and information. Senior Managers oversee data curation and management, and Operations support data population.

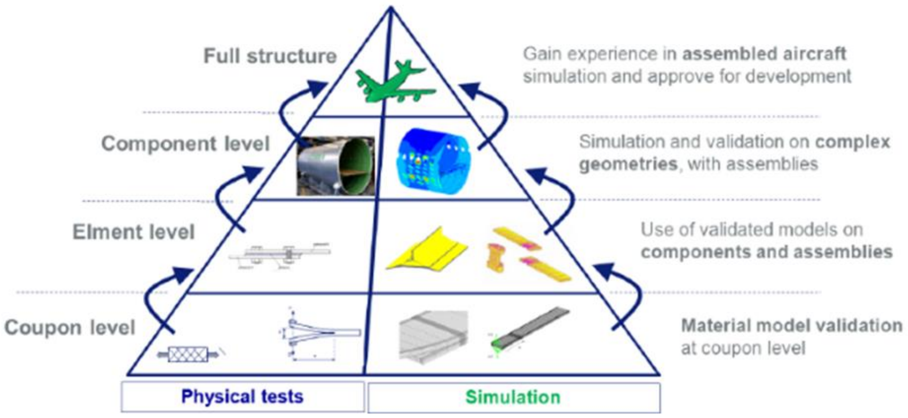


Figure 7: Building block approach to multi-scale modelling and validation testing, notably for aerospace composite structures [27]

Material models are evaluated based on acceptance criteria defined by quality measures set by either the Business Manager or Senior Manager, such as accuracy and reliability. Model candidates and outcomes are shared with the Business Manager, who may or may not need to have a deep understanding of the candidate models selected. The decision-making tool to select material models and ensure traceability may range from a spread sheet, a documented discussion/presentation of options between key internal/external stakeholders, a fully automated tool, a project management tool (e.g. JIRA), a dashboard, or a combination of these tools depending on the sector requirements for traceability, budgets and the project/program team. The model selection process is depicted in this work as dashboards which are commonly used in material and part selection processes for aerospace and automotive design projects, notably for formal *stage-gate* project management processes as defined by BDSS end-users in the FORCE and COMPOSELECTOR projects (the figure below provides a crude representation, whereas more refined examples are included in the BDSS IMPLEMENTATION section).

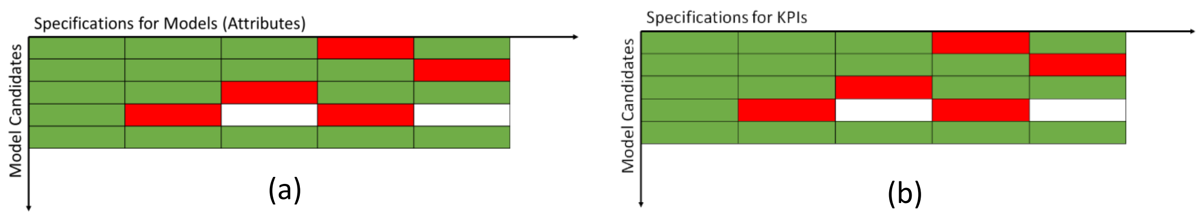


Figure 8: Dashboard concept for the selection of material models against (a) model requirements, and (b) business KPIs

4 BDSS TOOL IMPLEMENTATIONS

The remainder of this work presents the methodology behind the BDSS-tool implementations generated within the FORCE and COMPOSELECTOR projects, along with User Cases to demonstrate the application of the BDSS[2]. The BDSS descriptions are using the vocabulary presented in the Terminology and Context sections.

4.1 COMPOSELECTOR BDSS Overview

Table 4: BDSS-tool Overview – COMPOSELECTOR

1. BDSS-tool Description (7 Components)
i) Decision-making strategy: for model selection is based on Business/User Case objectives follows the following steps: • the Business Manager uses a **dashboard** of KPIs for comparison of product concepts. The KPI values are informed by model outcomes for technical performance of the material and/or part, and applications related to NPV, cost, time, sustainability and business risk; • the Senior Manager uses a combination of **visualization** and **multi-criterion optimization** (MCO) tools to select the model, or modelling workflow, best suited for a product concept depending on a detailed analysis of parameter sensitivity, model complexity, and uncertainty quantification. The workflow of KPI to model selection is the same as described in Figure 4. • the Operation personnel uses an **information management interface** and **open simulation platform (OSP) interface** which together enables data management, simulation workflow creation and execution (including material, process and part simulations), access to approved experimental data for validation, and the modelling/simulation requirements for the User Case. Experts from various Business Entities are required to fulfil information related to technical performance, manufacturing process, NPV, cost, time, sustainability and risk of the material/process/product. Verification activities for in-house code development are also supported by the information management interface. • The strategy is executed with a specific constellation of interoperable software tools with multiple interfaces depending on the stakeholder, their level of utility with materials models and business information, and their domain expertise. The tools are made interoperable to ensure traceability of decision-making and a shared source of data/information.
ii) Expertise needed on: fibre reinforced polymer (FRP) composite materials (including constituents), design, manufacturing, modelling and simulation, business process modelling, design and optimization, uncertainty management, data management, interoperability.
iii) Computational tools chosen: At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. eXstream DIGIMAT MF and

[2] **Please contact the EU project coordinators directly for more details about availability of the solutions for in-house purchase.**

DIGIMAT-FE, ESI PAMFORMVPS and PAM-RTM tools, Politecnico di Torino MUL2, mesoscopic modelling tool COMSOL used by INSA Lyon, LIST CmbsFE, ComPoSTE, Abaqus Simulia, LAMMPS used by University of Trieste.
iv) Experimental data: used for input parameters, verification, validation activities available to the end-user via the GRANTA MI materials information management system.
v) Data/Information management: experimental and simulation data is handled by GRANTA MI materials information management system. Data related to NPV, cost, sustainability and risk assessments of materials, processes and product concepts are managed in GRANTA MI.
vi) Traceability: The BDSS architectural diagram for interoperability is illustrated in Figure 10 and consists of three layers: i) Business Layer (CARDANIT); ii) Materials Information Management Layer (GRANTA MI); iii) Simulation Layer (MuPIF) within which the computational tools are denoted as Code 1, 2, etc. Traceability of decisions and data sources is supported by the CARDANIT tool for the high-level workflows for business processes (implementation of DMN and BPMN standards); simulation workflows are hosted in GRANTA MI; decision-making tools for NPV, cost, sustainability and risk assessments are traceable from GRANTA MI applications.
vii) Quality assurance: D8.5 Software Quality Management Report (see CORDIS)
2. BDSS-tool Attributes
2.1 Value Proposition for the BDSS-tool itself
Main Benefits (see Appendix A for a full listing of potential benefits): Reduced cost and risk to product development; product improvements; reduced time-to-market.
Business Entities whose aspects have to be taken into account in the BDSS: Finance/Procurement, Regulations, HSE, IT, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources).
Product Life Cycle Phases to be incorporated in the application of the BDSS: concept design, manufacturing process, detailed design
Reasons to include Simulation in the BDSS (sweet spots, see INTRODUCTION): ii) characterising a material system; iii) understanding effects of processing on properties; iv) screening hypothetical new materials; v) enabling computer-aided design; vi) facilitating substitution (e.g. due to REACH legislation).
Attributes of all of the above aspects to be taken into account by the BDSS tool: Manufacturability (cure time, % reject, volume), Mechanical (yield stress, specific strength, shearing strength, bending strength, compressive strength, tensile strength, hardness, young's modulus, Poisson's ratio, storage modulus, loss modulus, damping factor), Chemical (composition, flammability, corrosion, alkalinity), Physical (density, electrical conductivity, thermal conductivity, specific heat capacity, thermal expansion, thermal diffusivity, glass transition temperature), Sustainability (CO_2, manufacturing waste, embodied energy, water, end-of-life), Risk (restricted substance-related regulations, safety), Economic (Cost, NPV), VVUQ (accuracy, complexity, cost, time, uncertainty, reliability, sensitivity).
2.2 User Experience on the BDSS-tool
The BDSS is being tested against three User Cases for end-users at DOW, AIRBUS and GOODYEAR. Stakeholder survey results will be released towards the end of the project.
2.3 Technology of BDSS-tool implementation
The BDSS solution enables FAIR treatment of data and information through various technology advances provided by leading commercial software organisations and research institutes, including (not limited to): Maintainability, Interoperability, Security, Access Control, Authentication, Workflow.

2.4 Economics of the BDSS-tool
Market: the solution is primarily aimed at Large Enterprises due to the high degree of automation, coordination of many tools and experts across domains, and traceability capabilities. The constellation of tools and/or the methodology could also be used for consulting to SMEs, but it is unlikely to be affordable by SMEs.
Cost of the BDSS tool: of implementation and maintenance includes i) licenses to software (DIGIMAT MF, VPS GRANTA MI, CARDANIT, ModeFrontier); ii) information technology (IT) support; iii) expertise (labour) to manage the modelling, experimental, decision-making workflows; iv) experimental data for validation; v) hardware; vi) training; vii) HPC. Tools such as MUPIF and LAMMPS are open source. MUL2, CADRAL, NPV and Costing tools are still in licencing discussions.

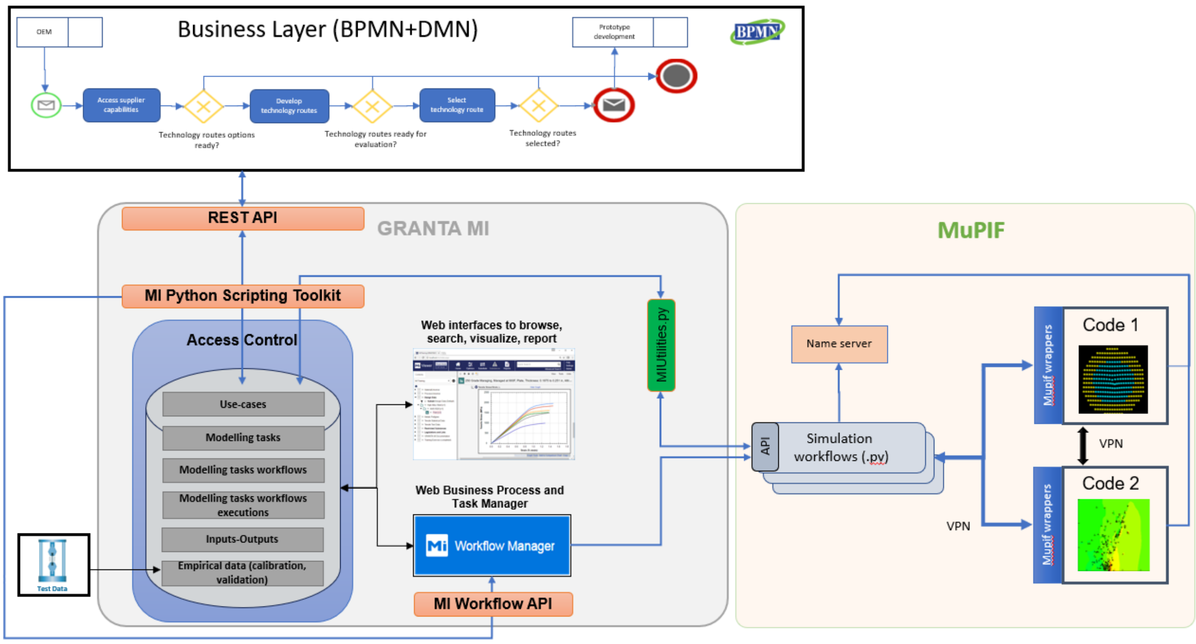


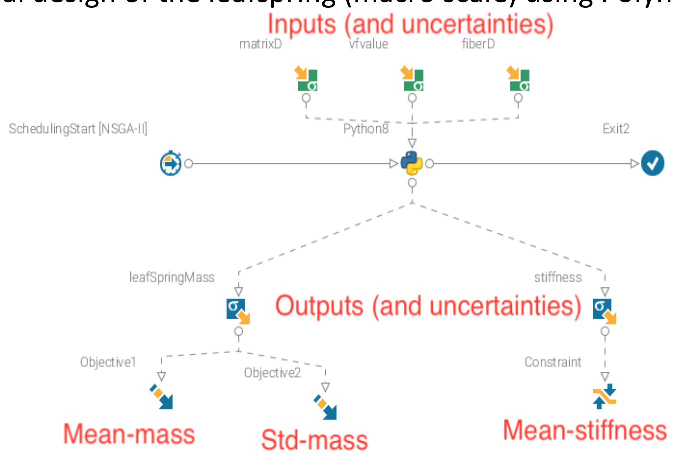
Figure 9: The COMPOSELECTOR BDSS platform

The Materials Layer (GRANTA MI), interacts with the Business Layer (CARDANIT) via MI:Workflow, and interoperates with the Simulation Interoperability Layer (MuPIF) and actual simulation codes by APIs. The end-user can consume stored data stored in the Materials Layer, request the generation of new data via the Business Layer, and ensure data is structured and appropriately stored for input/output to each simulation workflow execution via the interoperability between the Materials and Interoperability Layers.

4.1.1 COMPOSELECTOR Leaf-Spring User Case

Table 5: BDSS User Case Information and Solution Approach - COMPOSELECTOR Leaf-Spring

User Case	Material selection for light-weighting an automotive leaf-spring  Hyperco Composite Leafspring
End-User	DOW
Business Objectives and Targets	▪ Lightweight the leaf-spring part, 10-20% of overall part weight (reduction of weight by 10% reduces fuel consumption by 7%, saves €1.6-6.5/kg material)
Business Entities	Finance/Procurement, Regulations, HSE, IT, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources)
Stakeholders	i) Engineer/Scientist (Business) Manager; ii) Materials Engineer/Scientist; iii) Process/Manufacturing Engineer; iv) Structural Engineer
Material Options	▪ Epoxy I: Longer Cure; Higher mechanical properties (Aromatic Amines) ▪ Epoxy II: Medium Cure, Medium mechanical properties (Cycloaliphatic Amines) ▪ Epoxy III: Faster Cure: 15 min cure time; Lower mechanical properties (Aliphatic Amines) ▪ Hardener: is mainly used to cure the epoxy resin, which causes a chemical reaction without changing its own composition. The curing time mainly depends on the hardener and epoxy mixing ratio. Formulation baseline: 1:1 (resin–hardener ratio) ±10% ▪ Fibre: Glass (3 options), Carbon (3 options)
Manufacturing Processes	Polymer rheology, textile compaction, infusion, curing
Material/Product/ Process Attributes	Density, strength, stiffness, cost, end-of-life (e.g. recycling, reuse, remanufacturing), cycle time, NPV, REACH
Constraints	Recyclable, geometry (length to fit within existing system), stiffness, elongation (limited according to the User Case failure requirements)
Material/Product/ Process Free Variables	Material (resin, percent filler, sizing, thermal conductivity, viscosity, glass transition temperature), geometry (thickness, width)
KPI	Part Mass (decrease by 10-20%), Part Stiffness, Cycle Time, Part Cost, NPV, REACH (must comply). Table 6 shows the Business Manager's Dashboard with targets, requirements for the KPIs.

Decision Criteria	Minimize (density, cost, cycle time), maximize (strength, NPV)
Trade-off Criteria	Business Manager discretion (KPIs, emerging regulations, product portfolio, market trends, risk, etc.) – criteria is not necessarily managed by the BDSS, for example REACH risk, which has a TRUE/FALSE KPI value.
Computational Tools and Model Types	At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. Model 1: Atomistic (Molecular Dynamics - MD); Tool: LAMMPS Model 2: Mesoscopic (Dissipative Particle Dynamics - DPD); Tool: LAMMPS Model 3: Continuum (solid mechanics of resin & nanofiller + fibers); Tool: Digimat-MF, Digimat-FE Model 4: Continuum (solid mechanics for thermoforming); Tool: COMSOL Model 5: Continuum, (fluid mechanics impregnation); Tool: PAM-RTM Model 6: Continuum, solid mechanics of curing; Tool: PAM-RTM Model 7: Continuum, solid mechanics of final component; Tool: MUL2
MODA	The workflow as depicted in the MODA is given in Figure 11 (see also MODA Chapter 1.5, available on CORDIS, T1.1).
Multi-Criterion Optimisation	No. of material options considered: 18 No. of process combinations considered: 1 No. of modelling workflow: 7 Total No. of optimization variables: 7
Uncertainty Quantification	ModeFRONTIER optimisation software is used for the stochastic analysis and uncertainty quantification. The uncertainties are propagated from the micro-scale to macro scale. The effect of these uncertainties is estimated on the final design of the leafspring (macro scale) using Polynomial Chaos.  *Figure 10: Workflow for uncertainty propagation and quantification for the Leaf-spring use-case. All inputs and outputs are connected with APIs. Design variable is defined as input. Objective and constraints are connected to outputs and the Optimizer*
Simulation Outcomes	Modelling Optimisation Outcomes and Workflow Selection, MCO results (to be added in a later release of this document)
Business Decision Outcomes	Business Manager's Dashboard for Material Selection (to be added in a later release of this document; refer to the Dashboard for the AIRFRAME User Case as an example)

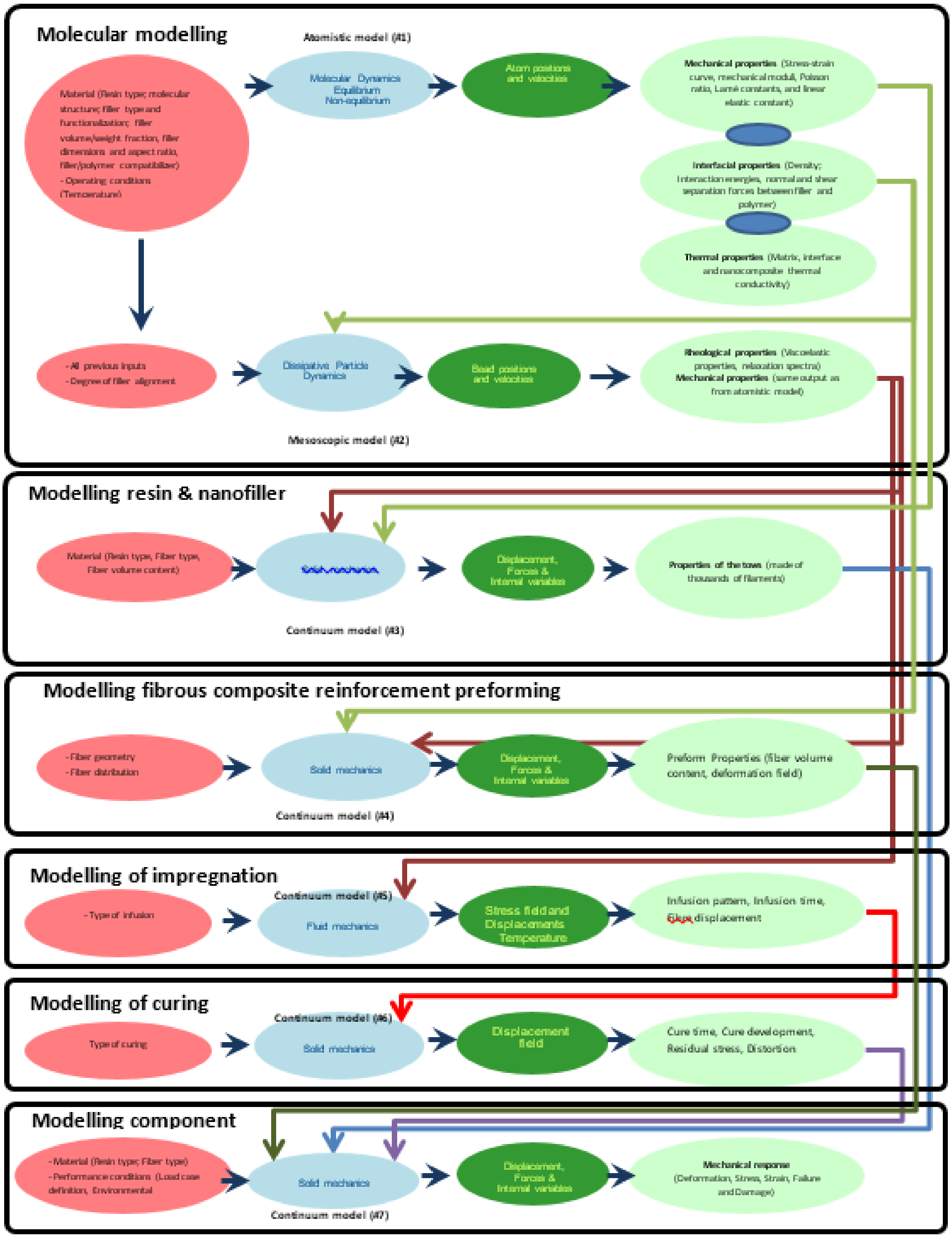


Figure 11: Modelling workflows for the Leaf-Spring User Case (part of the MODA description of the simulation)

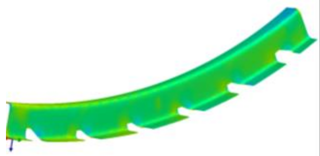
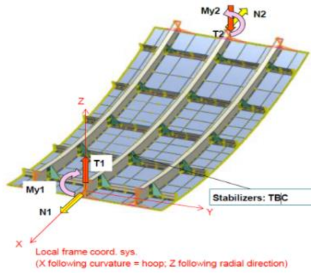
Table 6: Business Manager's Dashboard - COMPOSELECTOR Leaf-Spring Component

KPI	Unit	Target Performance	Minimum Acceptable Performance	Importance	Linked to KPI	Concept 1		Concept 2	
						Value	Uncertainty	Value	Uncertainty
Part Mass	kg	4.5	4.8	High	Cost, NPV	4.2	+/- 5%	4.7	+/- 5%
Part Stiffness	N/mm	300	285	High		310	+/- 5%	290	+/- 5%
Cycle time	sec	280	300	High	Cost, NPV, Part Mass	280	+/- 8%	283	+/- 8%
Part Cost	Euro	50	52.5	Critical	Cycle Time, Part Mass, NPV	53	+/- 7%	44	+/- 7%
NPV	Million euro	5	4	High		4	+/- 10%	4.6	+/- 10%

Note: a traffic-light representation (green, yellow, red) has been applied against the values for the concepts (design concepts), indicating acceptance or failure against the Target Performance

4.1.2 COMPOSELECTOR Airframe User Case

Table 7: BDSS User Case Information and Solution Approach - COMPOSELECTOR Airframe Component

User Case	Material selection of an Airplane Fuselage Airframe (Frame component)  
End-User	Airbus
Business Objectives and Targets	▪ Integrated: targeted production rate: 60 AC/month (±10) ▪ Costing: The objective is to reduce the cost of the finished component by roughly 20% when compared to the existing one. 20% cost reduction (current baseline 380 €/kg on thermoset frames) ▪ 10% of weight reduction ▪ Same technical performance as existing one: buckling Loading, stiffness as existing one (130 GPa) ▪ 10% Cycle time decrease (To be aligned with production rate) ▪ 20% increase use of recycling materials
Business Entities Providing Data/Information	Regulations, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources), Life Cycle Engineering
Stakeholders	i) Engineer/Scientist (Business) Manager; ii) Materials Engineer/Scientist; iii) Process/Manufacturing Engineer; iv) Structural Engineer
Material Options	▪ PEEK (Baseline Solvay): semi-crystalline thermoplastic, excellent mechanical and chemical resistance properties, highly resistant to thermal degradation, organic and aqueous environments. ▪ PEKK (Arkema Kepstan 7002): Semi-crystalline, excellent mechanical and physical properties, high processing temperature, expensive. ▪ Semi-finished product (UD Tape) is provided by Toho Tenax: UD Tape 12” or Slit tape 1/4’’. Fibre areal weight (FAW): 194gsm. Resin content: 34%. They are impregnators: they manufacture UD Tape by melting Carbon fibers and PEKK polymer. ▪ Semi-finished product: Still under development. No commercial datasheet available. Confidential data will be communicated by Airbus. ▪ CNT-Reinforced PEEK or CNT reinforced PEKK. ▪ Fibres and reinforcements: Mainly carbon fibres – woven, non-crimp, random, combinations of different types (surface weight, fibre orientations, etc.). Different sizing chemistry to maximize interfacial strength between fibre and matrix, ultimate strain, no. of filaments, etc.

Manufacturing Processes	▪ Pultrusion: Pultrusion is an additive manufacturing technology that integrates reinforcement impregnation with composite consolidation. The reinforced fibres (in the form of tape, woven, and/or mat) are driven through a thermoplastic resin bath. ▪ Thermoforming: Process converting a sheet to a three-dimensional part. ▪ AFP: AFP is an additive manufacturing technology for composites. It consists in an automated manufacturing process of heating and compacting resin pre-impregnated fibres.
Material/Product/ Process Attributes	Density, strength, stiffness, buckling, weight, cost, end-of-life (e.g. recycling, reuse, remanufacturing), cycle time, NPV, REACH
Constraints	Recyclable, geometry, stiffness, strength, buckling, time cycle, cost, weight
Material/Product/ Process Free Variables	Material (reinforcement (UD, Prepeg., etc.), matrix (PEEK, PEKK, …), geometry (thickness), processing technology (forming, injection, etc.)
KPI	Part mass, part stiffness, strength, buckling load, manufacturing, cycle time, part cost, NPV REACH (must comply). A similar dashboard format to Table 6 was agreed for the Airframe User Case but is not added to this description due to confidentiality of KPI requirements and targets.
Decision Criteria	Minimize (mass, cost, cycle time), maximise (strength, stiffness and buckling load, NPV)
Trade-off Criteria	Business Manager discretion (KPIs, emerging regulations, product portfolio, market trends, risk, etc.) – criteria is not necessarily managed by the BDSS
Computational Tools and Model Types	At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. Model 1: atomistic for polymeric matrix/filler interfacial properties, and system equilibrium density; Tool: LAMMPS Model 2: mesoscopic for rheological properties of the polymer matrix and filler-loaded composite; Tool: LAMMPS Model 3: continuum, micro-mechanics, to compute effective mechanical properties; Tool: DIGIMAT-MF (and DIGIMAT-FE) Model 4: continuum, mechanical macroscopic stress and strain fields; Tool: COMSOL Multiphysics Model 5: continuum, structural analysis of the final part; Tool: MUL2 Model 6: continuum, structural analysis of the final part; Tool: ESI Virtual Performance Solution (VPS)
MODA	The modelling workflow as given in the MODA is represented in Figure 12 (see also Chapter 1.5 of the MODA, available on CORDIS, T1.1).
Multi-Criterion Optimization	No. of material options considered: 10 No. of process combinations considered: 3 No. of modelling workflows: 7 Total No. of optimization variables: 6
Uncertainty Quantification	ModeFRONTIER is used for the stochastic analysis and uncertainty quantification. The uncertainties are propagated from the micro-scale to macro scale. The effect of these uncertainties is estimated on the final design of the airframe and reinforcing materials (macro scale) using Polynomial Chaos.

Simulation Outcomes	Modelling Optimization Outcomes and Workflow Selection, MCO results (to be added in a later release of this document)
Business Decision Outcomes	Business Manager's Dashboard for Material Selection has been added and will be updated in a later release of this document.

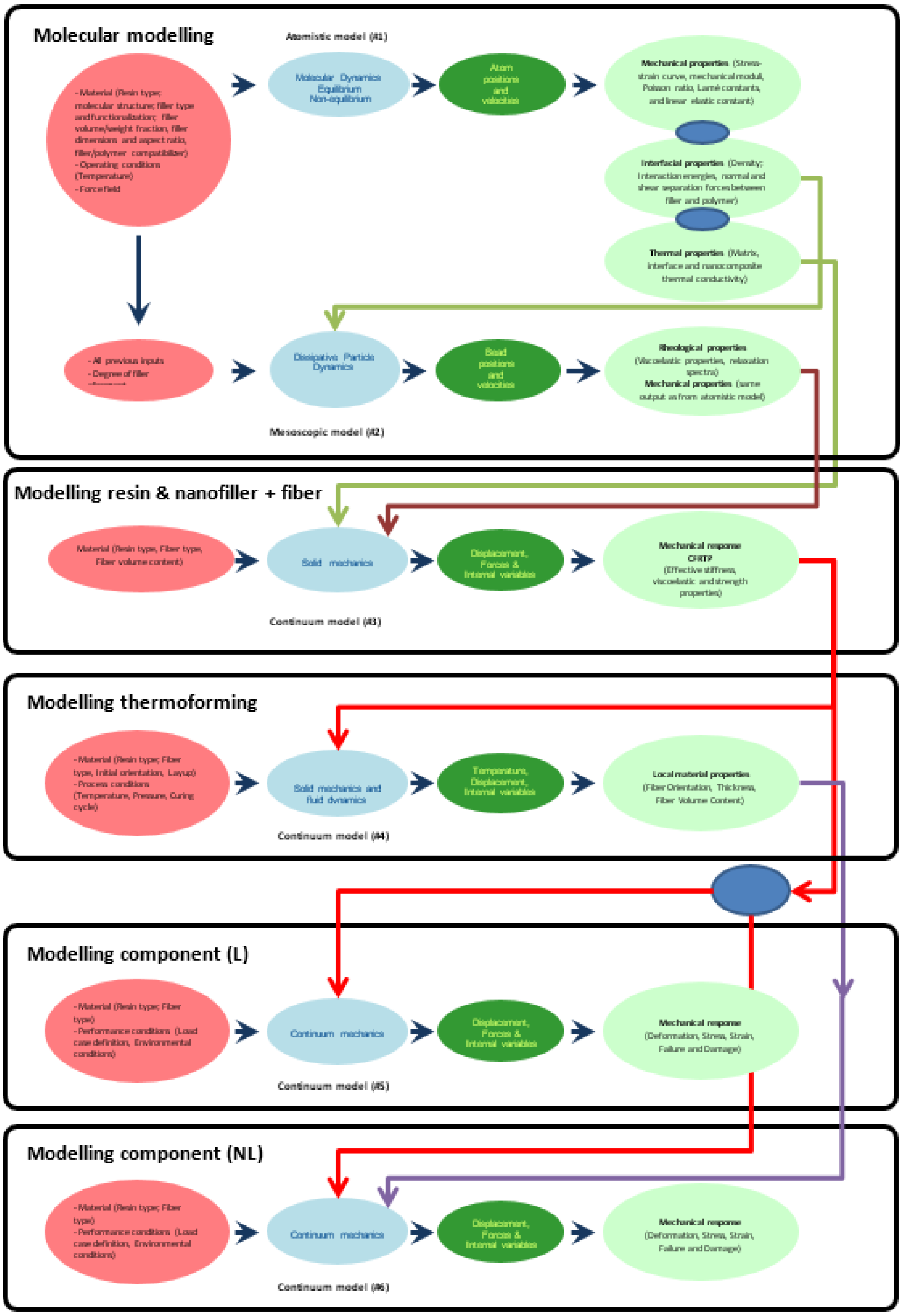


Figure 12: Modelling workflows for the Airplane Fuselage Component User Case (part of the MODA description of the simulation)

4.2 FORCE BDSS Overview

Table 8: BDSS Overview - FORCE

1. BDSS Description (7 Components)
i) Decision-making strategy: the Force platform will be open access and based on standards such that all components (modelling, MCOs, KPIs, dataspaces, etc.) can seamlessly exchange relevant information allowing an optimal business decision workflow to be developed rapidly while the availability of cognitive elements in the user interfaces will allow use even by non-experts in the materials modelling. Data from modelling will be augmented with existing data including chemical and flow properties, process characteristics, commercial and business data. Information on costs of raw and compound materials, processing, market trends and customer needs and demands will be included. Decisions based on this variety of information will be facilitated by dashboards and multi-criteria-optimisation (MCO) tools. These tools are particularly useful to identify best compromises when dealing with conflicting objectives, which are typical in materials design (e.g. lighter-stiffer, cheap-high purity, etc.).
ii) Expertise needed on: chemical formulations
iii) Computational tools chosen: At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. continuum modelling tools (openFoam), atomistic modelling tools (Gromacs), simulation platform (Simphony with the FORCE BDSS WORKFLOW Manager), MCO tools (Dakota, ModeFrontier…), data-driven modelling tools (IBM Watson)
iv) Experimental data: used for input parameters, verification, validation activities made available to the end-user in the various database plugged in including GRANTA MI database system that is interoperable via the SimPhoNy Open Simulation Platform and with the ENTHOUGHT BDSS FORCE Workflow Manager.
v) Data/Information management: both simulation and experimental data is handled by the BDSS platform through plugins. GRANTA MI is the materials information management system hosting both experimental and simulation data, and interoperating with SimPhoNy via wrappers (supporting SQL, no SQL backend solutions). Other databases support specific software (IBM, ModeFrontier), and can also be interoperable with the BDSS framework. All data generated in FORCE is casted in an ontology based (EMMO compliant) common universal data structures that are maintained (curated) in the various backend data repositories connected with the FORCE system.
vi) Traceability: of decisions, simulation workflows, and data sources is supported by GRANTA MI and output of the BDSS workflow manager. The **BDSS architectural diagram** for interoperability is illustrated in Figure 13. Traceability is supported in part by ontology-based data structures and the various semantic aware data repository and data management backends.
vii) Quality assurance: To be updated in the next release of this document.
2. BDSS Attributes
2.1 Value Proposition
Main Benefits (see Appendix A for a full listing of potential benefits): Reduce production and operation costs, increase market-share by addressing Governmental/ Regulatory Requirements (e.g., Energy Class A++++, sustainability…), customer demands (shiny colour, low energy consumption), speed of decision making: ability to determine, in-silico, the suitability of new raw

materials or optimal composition of existing materials, without extensive experimental testing. Rationalization of technological development efforts, optimization of production.
Business Entities: using and/or enabling the BDSS - Finance (total raw materials cost), final product performance (foam part density, foam thermal insulation performance), IP Management (patenting, avoid litigation), Regulations, Marketing, Supply Chain Management, Product Development, Marketing.
Product Life Cycle Phases: concept design, manufacturing process, detailed design
Project Types (sweet spots): i) addressing open research questions; ii) characterising a material system
Modelling attributes: accuracy, complexity, cost, time to market, time to solution, time for modelling and experiment, uncertainty, reliability, sensitivity, TRL, validation status, verification status, needed expertise.
2.2 User Experience
The BDSS is being tested against three User Cases for end-users at DOW, Unilever and Megara.
2.3 Technology
The BDSS solution enables FAIR treatment of data and information through various technology advances provided by leading commercial software organisations and research institutes, including but not limited to: Maintainability, Interoperability, Security, Access Control, Authentication, Workflow.
2.4 Economics
Market: the full solution is primarily aimed both Large and small Enterprises providing versatile automation and coordination of many tools and experts across domains that can be customised and maintained to specific applications. The FORCE BDSS is not meant to be a general, out-of-the-box platform, but to provide a platform for creating highly customised solutions, hence it is well suited to SMEs or specific technological and business questions.
Cost: of implementation and maintenance includes i) licenses to software required for modeFrontier, GRANTA MI, Watson IBM; Tools such as openFoam, Gromacs, BDSS workflow manager are open source. Tool/app for MCO tools and SimPhoNy are BSD licensed though some parts may be subject to other licenses, i) information technology (IT) support; iii) expertise (labour) to manage the modelling, experimental, decision-making workflows; iv) experimental data for validation and training data-based models; v) hardware; vi) training. This BDSS does not include HPC requirements, although they should be added in most User Cases.

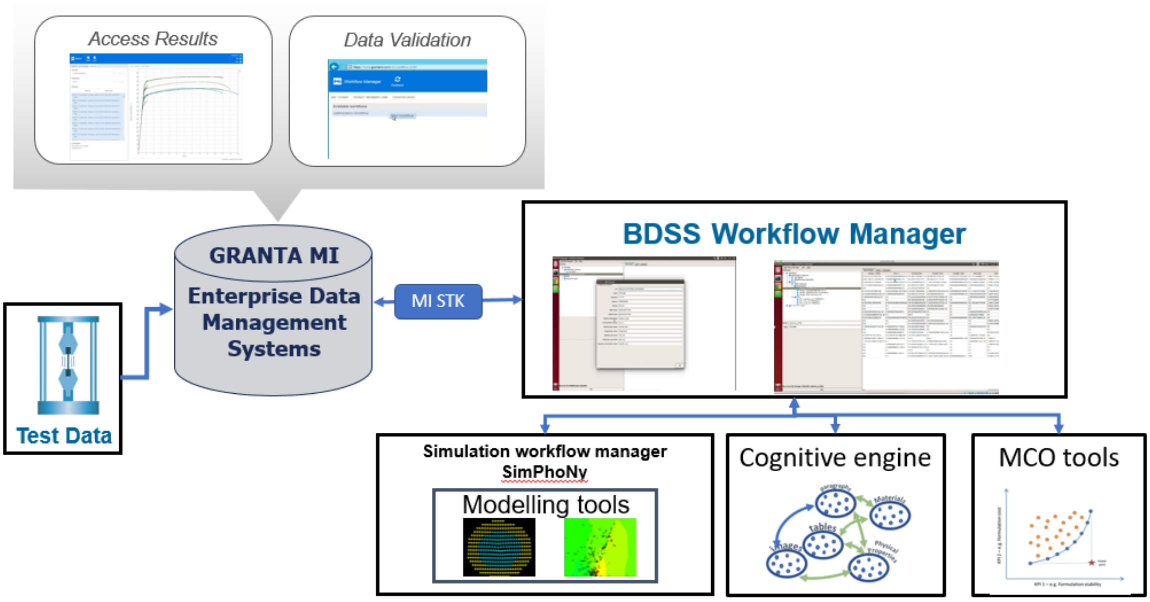


Figure 13: The Force BDSS platform

4.2.1 FORCE Personal Care Liquids Formulation User Case

Table 9: BDSS User Case Information and Solution Approach – FORCE Personal Care Liquids

User Case	Compliance with regulations for consumer segmented personal care fluids
End-User	Unilever
Business Objectives and Targets	▪ Assessment on whether a new surfactant can be used as a replacement in shampoo formulation for enhanced performance and agreeable costs.
Business Entities	Finance/Procurement, supply chain, Regulations, EHS (Environment, health and safety), IT, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources)
Stakeholders	i) Business Manager (project manager); ii) Formulation Scientist; iii) Process/ Manufacturing Engineer
Material Options	Confidential lists of possible surfactants and costs for shampoos
Manufacturing Processes	Not relevant.
Material/Product/ Process Attributes	Viscosity (Shear rate dependent), Salt concentration, size of micelles, price of materials, cost of performing the research (including costs associated with the BDSS software system, experiments, data, and time of personnel)
Constraints	Surfactant costs, supply chain
Material/Product/ Process Free Variables	Salt concentration, Concentration of individual surfactant or surfactant mixtures

KPI	▪ Size of micelles (target: >= 2000 surfactants per micelle) Viscosity (at 4.0 per sec) (Target: >= 10,000cP), ▪ Formulation cost (Target: Set by BDSS operator depending on current market requirements) ▪ Cost of simulation results ▪ High familiarity with modelling tools and models (to lower the cost of the simulations). Table 10 shows the Business Manager's Dashboard with targets, requirements for the KPIs.
Decision Criteria	▪ Average micelle size must exceed target size ▪ Maximum viscosity must be higher than a target viscosity ▪ Formulation cost must not exceed project target
Trade-off Criteria	Business Manager discretion (KPIs, emerging regulations, product portfolio, market trends, risk, etc.) – criteria is not necessarily managed by the BDSS
Computational Tools and Model Types	At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. Model 1: Mesoscopic (Coarse grain Molecular Dynamics); Tool: Gromacs Model 2: Atomistic (Molecular Dynamics); Tool: Gromacs
MODA	Figure 14 provides a screen shot of the down-selection app. The modelling workflows for the Printing Inks User Case are illustrated in the MODA in Figure 15 (also see Chapter 1.5 of the MODA, available on CORDIS, D1.2). As stated by the MODA authors, this figure represents the simulation of the rheology of liquid formulations, a consecutive workflow with an extension to include interlinked coarse-grained models with validation.
Multi-Criterion Optimization	No. of material options considered: ~12 ingredients and ~10-1000 combinations No. of process combinations considered: 1 (simple mixing) No. of modelling workflow: 3 No. of KPI considered: 3 Total No. of optimization variables: up to ~5 (surfactants concentration)
Uncertainty Quantification	Estimates based on comparison to some reference experiments, standard deviations from the trajectories of same run and from different initial conditions (from atomistic molecular dynamics trajectories).
Simulation Outcomes	Workflow selection is supported by storying relevant information in GRANTA MI. The user can selecte simulation workflows from the MI: Explore app (Figure 14). Selection can be based on various criteria such as: time to solution, target properties (Viscosity curve, viscosity at specific shear rate, micelle size distribution, variation of cell size), needed expertice, available software, target accuracies etc. Simulation KPIs can be incrementally added as needed. Outcomes are stored in GRANTA MI and can be explored in the same app.
Business Decision Outcomes	Best base solutions for next stage of development (first Gate for using a new ingredient in a Stage-Gate paradigm), including pricing information as well as technical details. Table 4.10 shows details of a Business Manager's Dashboard for the Stage-Gate process explored for this User Case.

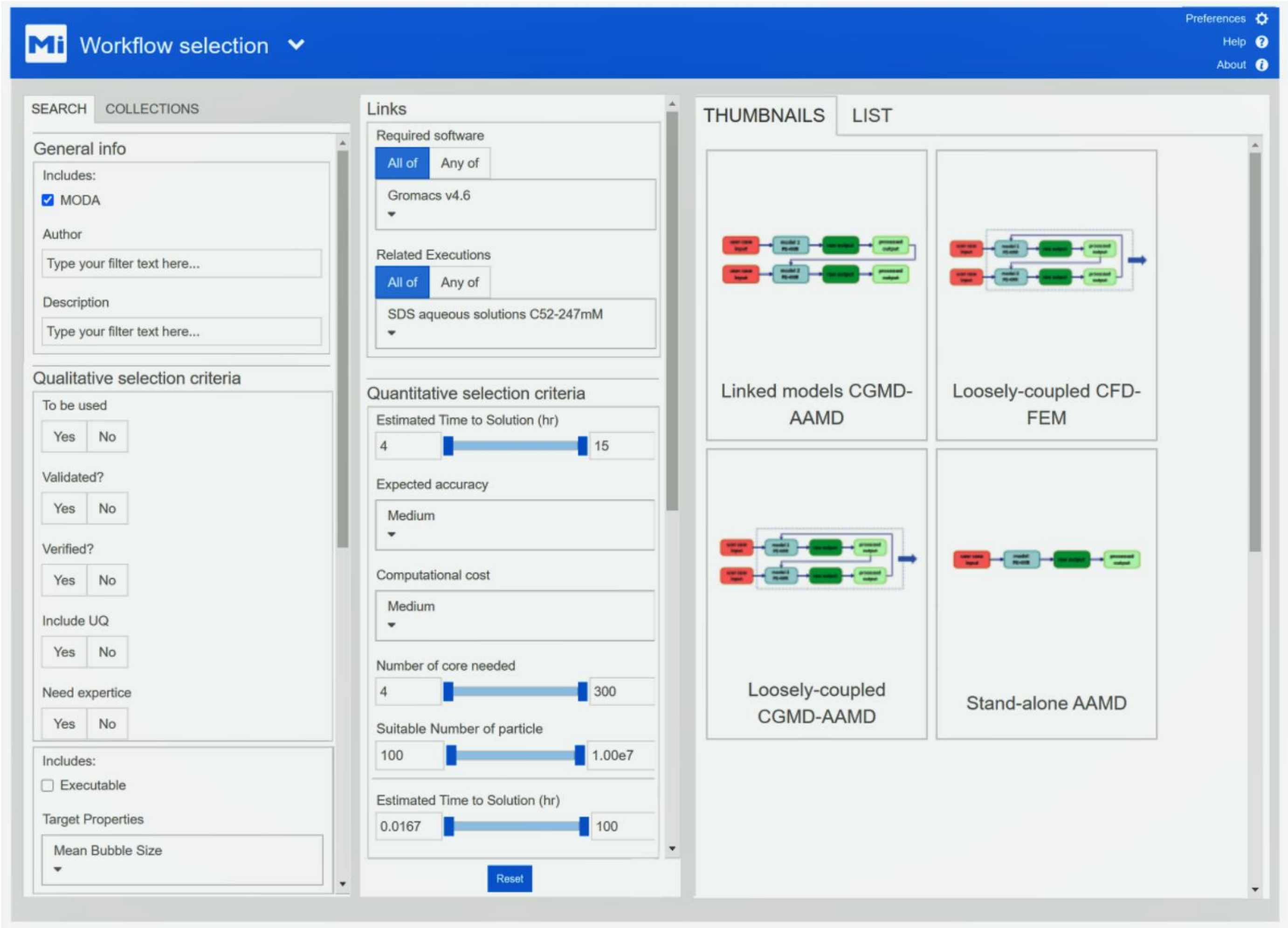


Figure 14: FORCE modelling workflow and selection strategy tool. Dedicated databases of records representing simulations, including requirements, objectives and outcomes.

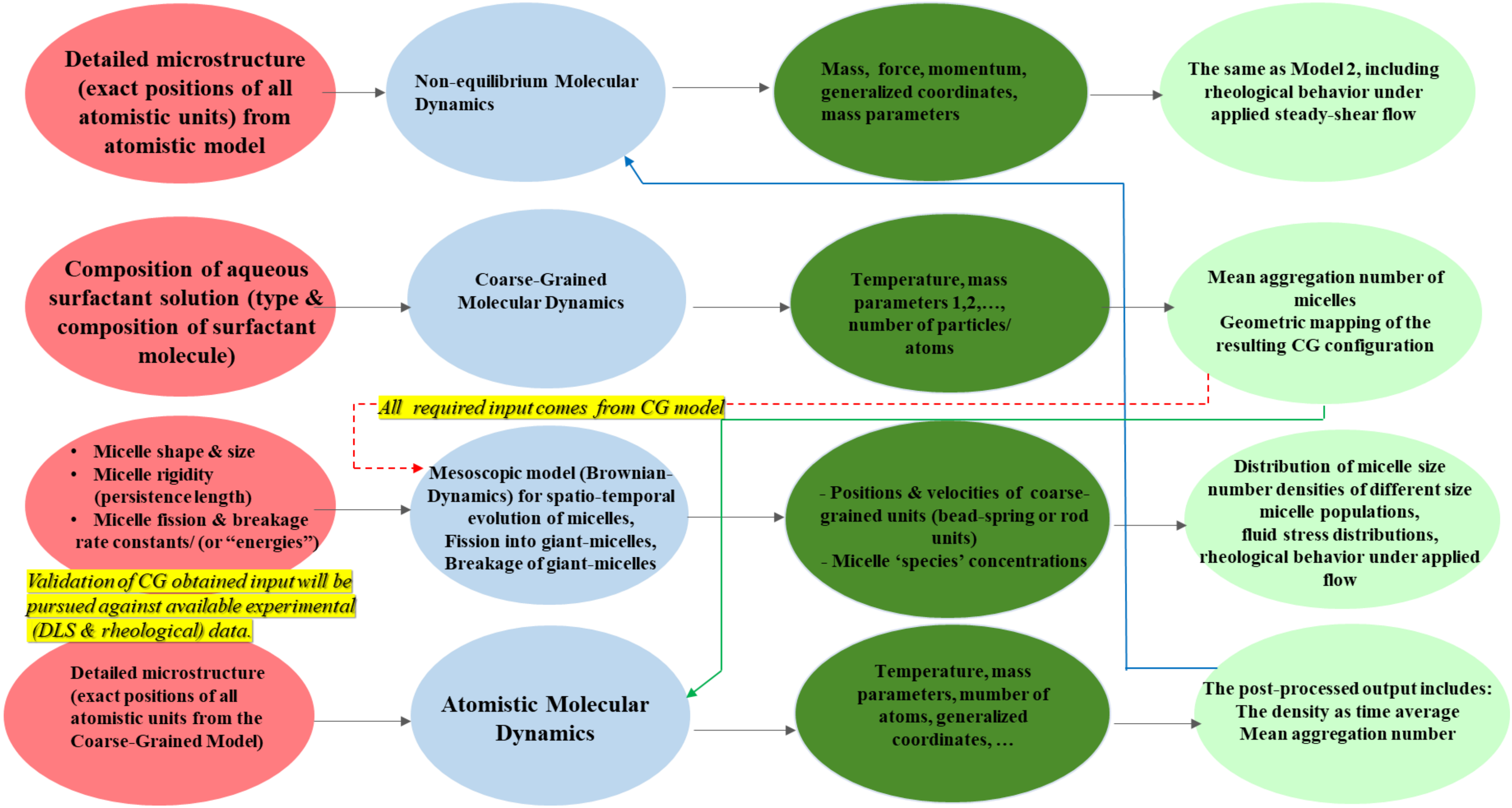


Figure 15: Modelling workflows for the Personal Care Liquid User Case (part of the MODA description of the simulation) that is a result of the BDSS process

Table 10: Business Manager's Dashboard – FORCE Personal Care Liquids (top 3 material candidates)

KPI	Actual Value	Unit	Target Value	Actual Uncertainty	Unit	Target Uncertainty	Importance of meeting KPI	Linked to KPI
Average Micelles size	[1]NA	surfactants per micelle	> 2000	NA	surfactants per micelle	45%	Medium	Viscosity
	NA			NA				
	NA			NA				
Formulation Cost	[2]CO	€/Ton	< 200 (depends on project)	CO	€/Ton	NA[3]	High	Cost
	CO			CO				
	CO			CO				
Viscosity	CO	[3]cP	> 10,000 cP	CO	cP	10%	Low	NA
	CO			CO				
	CO			CO				

[1]NA: Not Applicable; [2]CO: Confidential; [3]cP: centipoise

4.2.2 FORCE Printing Inks Formulation User Case

Table 11: BDSS User Case Information and Solution Approach – FORCE Polyurethane Printing Inks Formulations

User Case	Reduce cost of production by controlling waste, comply better with environmental regulations, and achieve customer target performances. More generally, optimisation of the production of Polyurethane (PU) based formulations for printing inks to be used on laminated products and flexible packaging applications and support for the development of new product segments.
End-User	Megara Resins
Business Objectives and Targets	Achieve zero waste production process, sustainable both economically and environmentally. Enabling control of the molecular weight of the PU variant by a data-based model is key. By controlling speed of agitation, temperature, water content, isocyanate content against final molecular weight, viscosity, grid formation, haziness and costs. Off-spec. batches are waste that increase the overall costs of the production.
Business Entities	Finance/Procurement, supply chain, Regulations, EHS (Environment, Health and Safety), IT, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources)
Stakeholders	i) Product line Manager (at manufacturing scale); ii) Process/Manufacturing Engineer (at manufacturing scale); iii) Research scientists (development of new products at lab scale)
Material Options	Confidential formulations and detailed reaction process sheets of polyurethane resins production.

Manufacturing Processes	Mixing in an industrial scale reactor. Detailed compositions of different reaction processes, characterized by a specific composition of the mixture and added materials, intermediate products, temperature, reaction duration and agitation speed.
Material/Product/ Process Attributes	Viscosity, molecular weight distribution of the final product, solid content.
Constraints	Raw material costs, production costs, production waste disposal and equipment cleaning (gelation), polyol purity (e.g. water traces) and dispersion index.
Material/Product/ Process Free Variables	Temperature, agitation and reaction times for each reaction step (3 to 10).
KPI	▪ Viscosity (Target: value dependent on product), ▪ molecular weight (Target: dependent on product), ▪ Total cost of production (Target: minimal), ▪ Total waste (Target: Zero) Table 12 shows the Business Manager's Dashboard with targets, requirements for the KPIs.
Decision Criteria	Optimum viscosity which should be within a specified range according to customer specs, curing time, creep behaviour, flow properties, (all according to customer needs), high flexibility of inks, film forming properties, adhesion and bond strength after fast curing on a variety of laminates, high compressive strength, good creep behaviour and low tack of nitrocellulose inks.
Trade-off Criteria	Business Manager discretion (KPIs, emerging regulations, product portfolio, market trends, risk, etc.) – criteria is not necessarily managed by the BDSS.
Computational Tools and Model Types	At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. Model 1: Data based model using machine learning Model 2: Continuum Kinetic Model
MODA	The modelling workflows for the Printing Inks User Case are illustrated in the MODA in Figure 16 (also see Chapter 1.5 of the MODA, available on CORDIS, D1.2).
Multi-Criterion Optimization	No. of material options considered: ~ 6-10 No. of process combinations considered: ~ 10 No. of modelling workflow: 1 No. of KPI considered: 3 Total No. of optimization variables: ~ 4
Uncertainty Quantification	UE ~ 20%, using variations from a machine learning model
Simulation Outcomes	Viscosity, gelation content (data-based model), molecular weight and solid content (physics-based models, reaction kinetics).
Business Decision Outcomes	Reaction Process, price and waste content. Note: Megara Resins is interested in a BDSS which would allow for shorter product development times for PU resins. The BDSS should be applicable to constant improvements within the existing product portfolio and for the development of new PU products not yet on the market.

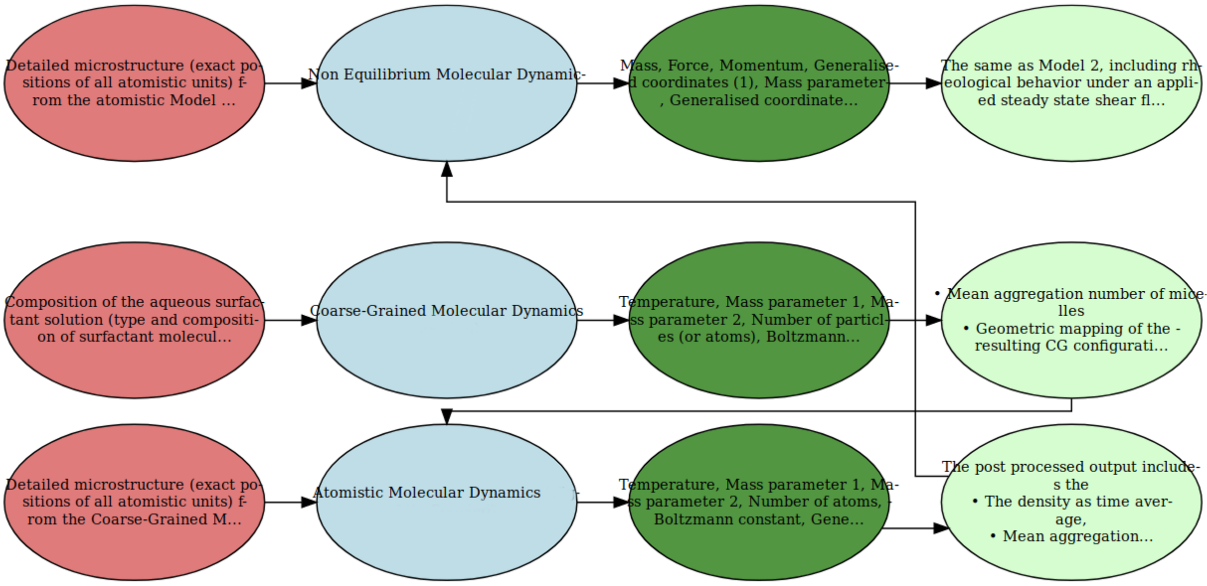


Figure 16: Modelling workflows for the Printing Inks User Case (part of the MODA description of the simulation)

Table 12: Business Manager's Dashboard – FORCE Polyurethane Printing Inks User Case

KPI	Actual Value	Unit	Target Value	Actual Uncertainty	Unit	Target Uncertainty	Importance of meeting KPI	Linked to KPI
Viscosity	1000 -1700 (Megapur RF 75)	mPa.s @ 20°C	1000-1700	NA	mPa.s @ 20°C	10%	high	Molecular weight distribution
Molecular weight distribution	Reference distribution plot (Mw < 15,000)	g/mol	According to reference distribution plot (Mw < 15,000)	NA	g/mol	10%	high	Viscosity
Total Cost	2.5 - 3	€/kg	<3	NA	€/kg	NA	high	Raw materials cost, production cost, amount of waste production
Solids content	75±1	%	75±1	NA	%	10%	high	viscosity

4.2.3 FORCE Foam Formulation User Case

Table 13: User Case Information and Solution Approach – FORCE Polyurethane Foam Formulation User Case

User Case	Deliver new PU FOAM formulation for latest isolation standard (e.g., A++++). This is essentially better compliance to support growth and market share.
End-User	DOW
Business Objectives and Targets	Produce PU system that will make molded rigid foam with low thermal conductivity (with a target value of less than 0.012 (W/(mK)) at a reduced cost. Cost and compliance driven decision.
Business Entities	Finance/Procurement, supply chain, Regulations, EHS (Environment, Health and Safety), IT, Product Development (Materials, Manufacturing Process, Structural, Product Design, Modelling & Simulation, Life cycle, Resources)
Stakeholders	i) Business Manager; ii) Formulation Scientist; iii) Process/Manufacturing Engineer;
Material Options	Confidential lists of possible components (of the order of 10 components per formulation as a minimum)
Manufacturing Processes	Mixing and blending, reactor, injection.
Material/Product/ Process Attributes	Foam density, mean foam cell size, raw material cost, component concentration, components selection (based on availability and cost of raw materials).
Constraints	Costs, choice of component available on given market given mold geometry, capacity of production lines.
Material/Product/ Process Free Variables	Component selection and concentrations, injected mass, component temperature, mold temperature and pressure conditions (ambient and mold).
KPI	Applied density (resulting mold density), k-value (thermal conductivity), cost of process and materials. Table 14 shows the Business Manager's Dashboard with targets, requirements for the KPIs.
Decision Criteria	▪ Foam thermal conductivity lower than the target value (KPI: k-value in W/mK) ▪ Molded foam density lower than the target value (KPI: Applied density in kg/m^3) ▪ Formulation cost lower than the target total raw material cost (KPI: Cost in €)
Trade-off Criteria	Business Manager discretion (KPIs, emerging regulations, product portfolio, market trends, risk, etc.) – not all criteria are necessarily managed by the BDSS but can be extended to include them as needed.
Computational Tools and Model Types	At the onset of the project selection criteria for models were not yet implemented and familiarity was the only attribute playing a role. Model 1: Continuum, CFD model (using OpenFOAM) with reactions and population balance equations (PBE) Model 2: A Fundamental thermal conductivity model (continuum)

	ModeL 3: Other optional supporting surrogate models (data-based models)
MODA	The modelling workflows for the Foam User Case are illustrated in the MODA in Figure 17 (also see Chapter 1.5 of the MODA, available on CORDIS, D1.2). Average size of micelles and (optionally) viscosity of surfactant system.
Multi-Criterion Optimization	No. of material options considered: 10 No. of process combinations considered: 2 (mass, temperature, flowrate) No. of modelling workflow: 1 up to 3 No. of KPI considered: 3 Total No. of optimization variables: up to 10
Uncertainty Quantification	Absolute error on minimal applied density (<15%) controlled by discretisation convergence studies.
Simulation Outcomes	Predicted Applied Density (minimum filling density needed to fill the mold cavity) Mean k-value of the foam Formulation cost
Business Decision Outcomes	Determine cost effective model to achieve desired Applied Density and k-value target. Accept business if the system cost returns a decided benefit.

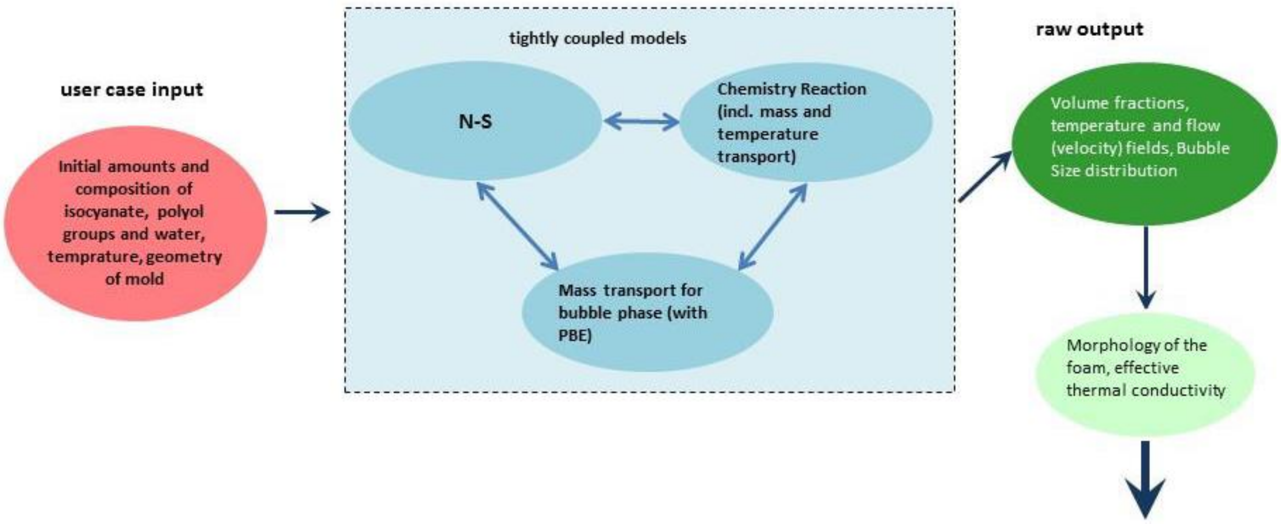


Figure 17: Modelling workflows for the Foam User Case (part of the MODA description of the simulation)

Table 14: Business Manager's Dashboard – FORCE Foam User Case Information

KPI	Actual Value	Unit	Target Value	Actual Uncertainty	Unit	Target Uncertainty	Importance of meeting KPI	Linked to KPI
Foam Thermal conductivity (k-value)	0.023	W/(m▪K)	<0.016	10	%	10%	High	Thermal conductivity (k-value)
Foam applied density	45	Kg/m3	<35	10	%	10%	High	Applied density
Formulation Cost	CO	€/kg	< 30 (depends on project)	CO	%	NA	medium	cost

5 RECOMMENDATIONS

The following recommendations are a starting point for future work:

1. With the release of this document, feedback and recommendations are welcome via the correspondence channel noted at the start of the document.

2. Wider dissemination of definitions of ROMM [7], CEN-CENELEC CWA 17284:2018 [8].

3. Demonstrate the modelling and simulation tool selection capabilities of the BDSS-tool

4. Establish strategy and benchmark case studies for VVUQ activities of materials modelling, along with a refined definition for ranking of *Complexity*.

5. Establish a management process for the Quality Assurance practices which are unique to materials model and simulation software developers, including concepts such as *Completeness* of the process and its associated information documentation.

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7 APPENDIX A: Business Benefits Related to Materials Modelling

EMMC-CSA Expert Meetings and Workshops, among other sources in the literature, have contributed to the following lists of benefits of materials modelling for manufacturing organisations [4, 28, 29, 30]. Benefits may be quantitative meaning comparable against a benchmark with a unit of measure (Table 15), or qualitative without a unit of measure (Table 16) and serve as a starting point for defining business objectives for material modelling.

Table 15: Quantitative benefits of materials modelling for manufacturing organisations

ID	Quantitative benefit
1	Saving stalled projects (solutions to design problems)
1.1	Estimate property data for materials that cannot be obtained for competitive reasons
1.2	Informed experimental design
1.3	Design innovation and quicker identification of materials
2	Improved functional performance for performance-driven materials
2.1	Structural concept developments for breakthroughs (e.g. weight, cost performance while maintaining safety)
2.2	Multifunctional structures (e.g. integrating wiring, systems, etc.)
2.3	Improved interface performance (e.g. lubricants, adhesives, coatings, bio compatibility, etc.)
2.4	Improved environmental resistance (e.g. corrosion, abrasion, wear)
2.5	Performance of functional materials (e.g. piezoelectric, photo voltaic, thermo-electric, etc.)
2.6	Long term technical performance (e.g. toughness and durability, fracture and fatigue, creep and stress relaxation resistance)
2.7	Improved aesthetics (e.g. improved surface classification)
3	Improved capabilities for predicting engineering system performance or life cycle.
3.1	Virtual engineering assessment of new materials that might be considered risky to assess with physical prototypes.
3.2	Virtual engineering assessment in systems where the validation of materials performance by system-level testing is expensive, time consuming, or not possible.
4	Faster and less costly new product development resulting in reduced time to market
4.1	High-through-put methodology and techniques
4.2	Integrated materials development, qualification, testing and certification in less time and with less cost compared with traditional methods
4.3	More efficient and targeted experimentation informed by modelling, saving time and cost of experiments
4.4	Lower cost to obtain certain property data (e.g. due to cost of experiment or synthesis)
5	More efficient (reduced) experiments
5.1	Combined modelling and characterization (replace experiments with computational results)
6	Innovation due to broader exploration
6.1	Increased market share, increased profit
6.2	Market advantage based on improved performance from incorporating materials and processes optimized for particular applications and on more precise modelling of a material's response to an application environment.

6.3	Higher margin product
6.4	Reduced costs of design and/or manufacturing
7	Improved control of the manufacturing process.
7.1	Improved production speed (optimization of production process)
8	Risk Management and improved resource efficiency
8.1	Less material waste and resources during R&D, manufacturing
8.2	Reduced environmental footprint (meeting regulations in some sectors; reuse/remanufacturing of waste or end-of-life product)
8.3	Avoid destructive testing
8.4	Avoiding potentially hazardous experimentation
8.5	Reduction of product failures during manufacturing, and after manufacturing
8.6	Reduced call back of bad product quality
8.7	Reduced supply chain risk (e.g. price volatility, restricted substances, environment, socio-economic drivers which trigger material substitution)

Table 16: Qualitative benefits of materials modelling for manufacturing organisations

ID	Qualitative benefit
1	Explore and adopt advanced methods and tools for integrated design
1.1	Enhance current suit of tools (match to current design time-frame)
1.2	Keep a watch on next generation analysis methods and tools
2	R&D strategy development
2.1	Improved insight and understanding of the processing and material properties from chemistry to application performance
2.2	Early, faster exploration by visualization of downstream applications, material behavior, formulation or process at multiple scales
2.3	Foster a culture of fail early, innovate faster
2.4	Solve problems which could otherwise not be solved
3	Grow and secure Intellectual Property claims
3.1	Discover, create and mature new material systems (IP generation and broader IP claims)
3.2	Support defensive IP publishing, i.e. pre-empt competition patents.
4	Communication and marketing via models and their visualization
4.1	Improve value chain interactions
5	New types of business: from Product to Product +, i.e. Product plus relevant "Model" (typically the relevant Materials Relations) to enable customer to build engineering models faster)
5.1	Avoid dead-ends in R&D
5.2	Ability to link materials chemistry/structure to application performance
5.3	Enables better informed decisions about material, product and processing choices
5.4	Avoid upscaling issues and lower risk of market introduction; reduction of product failures during manufacturing, and after manufacturing
5.5	Support trouble-shooting of material/product failures
5.6	Validation of supplier information
5.7	Build customer trust
5.8	Demonstrate competitive advantage via competitor materials based on models

8 APPENDIX B: Acronyms

AFP = automated fibre placement

API = application program interface

APP = application

ASME = American Society of Mechanical Engineers

BDSS = Business Decision Support System

BSD = Berkeley Software Distribution

CEN = Comité Européen de Normalisation (European Committee for Standardization)

CENELEC = Comité Européen de Normalisation Électrotechnique (European Committee for Electrotechnical Standardization)

CEO = Chief Executive Officer

CNT = carbon nanotubes

COMPOSELECTOR = Multi-scale Composite Material Selection Platform with a Seamless Integration of Material Models and Multidisciplinary Design Framework

COO = Chief Operating Officer

CORDIS = Community Research and Development Information Service

CSA = Coordination and Support Action

CWA = CEN Workshop Agreement

DPD = dissipative particle dynamics

E = error

EHS = Environment, Health, Safety (also HSE)

EMMC = European Materials Modelling Council

EMMO = European Materials Modelling Ontology

ERP = Enterprise Resource Planning

FAIR = Findable Accessible Interoperable Reusable

FORCE = Formulations and Computational Engineering

GA = Grant Agreement

IP = Intellectual Property

IT = Information Technology

KPI = Key Performance Indicator

LEIT = Leadership in Enabling and Industrial Technologies

MCO = Multicriteria Optimization

MD = molecular dynamics

MODA = Modelling Data

MR = Materials Relations

NAFEMS = National Agency for Finite Element Methods and Standards

NASA = National Aeronautics and Space Administration

NMBP = Nanotechnologies, Advanced Materials, Biotechnology, Advanced Manufacturing and Processing

NPV = net present value

PE = Physics Equation

PEEK = Polyetheretherkeytone

PEKK = Polyetherketoneketone

PI = Performance Indicator

PLM = Product Lifecycle Management

Prepreg = pre-impregnated

PU = Polyurethane

R&D = Research and Development

REACH = Registration, Evaluation, Authorisation and Restriction of Chemicals

ROI = Return on Investment

ROMM = Review of Materials Modelling

RTM = resin transfer molding

SAE = Society of Automotive Engineering

SME = small-and-medium-enterprise

SQL = standardized query language

TRL = technology readiness Level

UD = uni-directional

UQ = Uncertainty Quantification

V = variance

V&V = Verification & Validation

VP = Vice President

VVUQ = Verification Validation Uncertainty Quantification