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Materials modelling - Terminology, classification and metadata

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European foreword

This CEN Workshop Agreement (CWA 17284:2018) has been drafted and approved by a Workshop of representatives of interested parties on 2017-12-11, the constitution of which was supported by CEN following the public call for participation on 2016-12-16.

A list of the individuals and organizations which supported the technical consensus represented by the CEN Workshop Agreement is available to purchasers from the CEN-CENELEC Management Centre. These organizations were drawn from the following economic sectors: Advanced Technology, Chemical Engineering, Research & Development, and Materials Modelling.

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The final review/endorsement round for this CWA was started on 2017-10-03 and was successfully closed on 2017-12-03. The final text of this CWA was submitted to CEN for publication on 2018-01-04.

Below is a list of companies/institutions that endorsed this CWA:

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Introduction

It has been demonstrated in many individual cases that materials modelling is a key enabler of research & development efficiency and innovation and that the use of this technology can generate a huge economic impact.

Due to the huge variety and complexity of materials and the wide range of applications the materials modelling field consists of a number of communities. These communities have established different terminologies which typically focus on specific application domains and on particular types of models. As a result, a wide range of domain specific software codes have evolved. However, applications to industrial problems in advanced materials and nanotechnology require a strong interdisciplinary approach among these fields and communities. There is therefore a need to establish a common terminology (definition of concepts and vocabulary) in materials modelling.

A standardized terminology will improve future exchanges among experts in the entire area of materials modelling, facilitate the exchange with industrial end-users and experimentalists and reduce the barrier utilizing materials modelling. The common language is expected to foster dialogue and mutual understanding between industrial end-users, software developers, scientists and theoreticians. Standardization of terminology and classification has been identified as critical to collaboration in and dissemination of European research projects. In particular, standards will facilitate interoperability between models and databases. The standardization is relevant for an integrated technological development and brings benefits for industrial end-users due to simplified and much more efficient communication in the field of materials simulation.

The classification helps translators by translating industrial problems into problems that can be simulated with materials models. It assists workflow development where several models can interoperate in addressing a specific end-user question.

In the future, this standardized terminology and classification can be formalized into a taxonomy and an ontology of materials modelling. Such an ontology will form the basis for formal metadata development with which models and databases can be linked. These developments will further support efficient solutions for materials modelling and the communication, dissemination, storage, retrieval and mining of data about materials modelling.

1 Scope

This CWA includes definitions of fundamental terms for the field of materials modelling and simulation. Computational materials models in this CWA are understood to be physics-based models. This CWA does not include data-based models.

The definitions enable a classification of materials models. Using the entity and physics equation concepts, leads to a relatively small number of distinct materials models replacing the current situation of opacity of materials models and simulations that make the field hard to access for outsiders.

This CWA also provides a systematic description and documentation of simulations including the user case, model, solver and post-processor: the “materials MOdelling DAta” (MODA). This document seeks to organize the information so that even complex simulation workflows can be conveyed more easily and key data about the models, solvers and post-processors and their implementation can be captured. A template MODA for physics-based models is described in order to guide users towards a complete documentation of material and process simulations.

The CWA is based on the Review of Materials Modelling (RoMM) [1]. A MODA for data-based models can be found in the RoMM [1].

2 Normative references

There are no normative references in this document.

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

3.1
Entity
self-contained, internally frozen, structure-less representational unit of a material

Note 1: The modeller chooses to describe the material at a certain level of granularity and does this in terms of the behaviour of a set of entities.

Note 2: There are four types of entity, one for each of the four levels of granularity:

1) electron entity: a representation of an electron [SOURCE: IEV 113-05-18]

2) atom entity: a representation of an atom [SOURCE: IEV 113-05-20]

3) mesoscopic entity: a representation of a set of bounded atoms (e.g. group of atoms, molecule, bead, cluster of atoms, nanoparticle, grain)

4) continuum volume entity: a representation of the material bounded in a region of space within which the material is considered by the modeller to be described by the same set of properties

Note 3: Electron entities, atom entities and mesoscopic entities are chosen for discrete representations of the material. Continuum volume entities represent the material as a continuum.

Note 4: Any material can be described by any of the entity types.

EXAMPLE: The internal structure of a material can be described as an arrangement of electrons or atoms interacting with each other. Alternatively, the modeller may identify discrete grains as mesoscopic entities and model the behaviour (e.g. magnetism) of the material based on internal and external forces on grains. The detail of a granular structure can also be captured by partitioning the grain into different continuum volumes.

3.2
Quantity
property of a phenomenon, body or substance, where the property has a magnitude that can be expressed as a number and a reference

[SOURCE: ISO/IEC Guide 99:2007, 1.1.]

Note 1: A physics quantity is a physical property of a phenomenon, body, or substance that can be quantified by measurement.

Note 2: The behaviour of an entity can be described by more than one physics quantity (e.g. mass, charge, velocity and temperature).

Note 3: The modeller chooses properties of the entity to be used and chooses to assign values to them in order to model a certain physical behaviour of the material.

3.3
Physics equation
mathematical equation based on a fundamental physics theory which defines the relations between physics quantities of an entity

EXAMPLE 1: Newtons equation of motion defines the relation between mass and acceleration of an entity and forces acting upon it.

Note 1: The physics equation is generally an approximation to the fundamental physics theory.

EXAMPLE 2: The Navier-Stokes equation is based on Newton’s second law and makes certain assumptions to define the relation between velocity, density, pressure and stress of a continuum volume entity.

Note 2: The physics equation is by its nature generic and independent of the specific material represented and the physics equation is therefore widely applicable.

Note 3: The physics equation contains variables (i.e. physics quantities for which the physics equation is solved) and parameters (i.e. physics quantities for which the equation is not solved) that need to be specified. These parameters are often determined for classes of materials.

3.4
Materials relation
materials specific equation providing a value for a parameter in the physics equation

Note 1: A set of materials relations complements the physics equation.

Note 2: Only the combination physics equation and materials relations is a complete set of equations that is solvable.

Note 3: Materials relations provide values for the parameters of the physics equation. They are given for the (specific) material to be simulated either as values if the parameter is constant or as relations (functions).

Note 4: Physics quantities not appearing in the physics equation can appear in materials relations.

EXAMPLE: Relations for Hamiltonians, force fields, mesoscopic interaction potentials and constitutive equations are materials relations of electronic, atomistic, mesoscopic and continuum models, respectively.

Note 5: A materials relation is valid only for the class of materials for which it is formulated. This is a feature that distinguishes between physics equations and materials relations.

3.5
Physics-based model
solvable set of one physics equation and one or more materials relations

Note 1: The set of physics equation and materials relation(s) is also referred to as governing equations.

Note 2: The set of equations is mathematically solvable once suitable conditions (such as initial and boundary conditions) are specified.

3.6
Physical system state
values of the physics quantities for the collection of entities used to represent a material at an instant of time

3.7
Physics-based model types

3.7.1
Electronic model
physics-based model based on a physics equation describing the behaviour of electron entities

3.7.2
Atomistic model
physics-based model based on a physics equation describing the behaviour of atom entities

3.7.3
Mesoscopic model
physics-based model based on a physics equation describing the behaviour of mesoscopic entities

Note 1: If interactions between different types of entities (e.g. atoms and beads in nanoparticle growth) are modelled, the model is called hybrid.

Note 2: In some cases, the same physics equation is formally used to describe the interaction between different types of entities. The materials relations are different for each combination of two different types of entities. An example of such a hybrid model uses Newton's equation for the description of the behaviour of a system composed of atoms and beads mesoscopic entities). Different materials relations are required to describe the atom-atom, atom-bead and bead-bead interactions.

3.7.4
Continuum model
physics-based model based on a physics equation describing the behaviour of continuum volume entities

3.8
Multi-equation modelling
description of a system by means of a set of interconnected models

3.9
Multi-scale modelling
multi-equation modelling in which models are applied at different length scales

3.10
Solver
set of techniques used to numerically solve a particular physics-based model

Note 1: There is a strict separation between the concept of 'Model' and 'Solver'.

Note 2: Solvers typically require discretisation of space and time. Solvers for some discrete models only need discretisation of time (e.g. Verlet integration).

Note 3: Some solvers use fictitious particles (e.g. Smoothed Particle Hydrodynamics).

3.11
Pre-processing
operations preparing input data for a simulation

EXAMPLE: Calculating input values for properties from a (experimental or simulated) database.

3.12
Post-processing
operations on raw output of solvers without altering the physical system state

EXAMPLE: calculation of homogenised properties of a material

EXAMPLE: visualisation of the results

3.13
Stand-alone model
physics-based model whose input is provided by the user case and whose processed output is not used by any other model

Note: The workflow for a stand-alone model is depicted in Table 3.

3.14
Linking
sequential solution of the governing equations of two or more physics-based models, where the processed output of one model is used as input for the following model

Note 1: Linking leads to an open loop data stream.

Note 2: Longer, more complex connection structures are possible and as long as the flow is strictly one-way the connections are called 'Linking'. A model can e.g. be fed from more than one model or feed more than one model. Conditional branching is also possible, where a model A feeds model B or model C depending on the physical system state.

Note 3: The workflow for linking is depicted in Table 3.

3.15
Iterative coupling
iterative solution of the governing equations of two physics-based models, where the processed output of the first model is used as input for the second model and the processed output of the second is used as input for the first

Note 1: Each model has its own processed output.

Note 2: Iterative coupling leads to a closed loop data stream.

Note 3: Solution requires a certain number of iterations to reach convergence.

Note 4: More than two models can be coupled.

Note 5: The workflow for coupling is depicted in Table 3.

3.16
Tight coupling
concurrent solution of the governing equations of two physics-based models where the physics equation and materials relations of each model are collected and solved as a single system of equations

Note 1: Model inter-dependency is expressed through physics quantities appearing in more than one equation.

Note 2: Tight coupling leads to one single raw output for all models.

Note 3: The workflow for tight coupling of models is depicted in Table 3.

3.17
Simulation
complete set of activities to arrive at a calculated answer to a specific question

Note 1: This consists of elaborating the user case, establishing the relevant models and databases, the computation (including solving) and the post-processing.

Note 2: A graphical representation of a simulation can be given in a diagram and is called workflow (see Chapter 6). It depicts the relations between all parts of the simulation and in particular between different models, databases and their coupling/linking.

3.18
Materials modelling data (MODA)
documentation of a simulation

Note: The MODA relates to one simulation for a particular user case (and does not necessarily describe the wide capabilities of the models).

4 Symbols and abbreviations

MODA Materials modelling data

MR Materials Relation

PE Physics Equation

RoMM Review of Materials Modelling [1]

5 Classification of materials models

Based on the terms and definitions, a systematic classification of materials models is as follows:

Physics-based models are classified at the top level by the entity whose behaviour is described. At the top level there are four types (see 3.1).

Models are further classified (at the next level) by the physics equation. For each type of entity about six distinct physics equations have been identified. For a list of the specific models of each type, see the content list of the RoMM [1].

Further classification for each model using one particular physics equation can be done by the materials relations.

6 Documentation of simulations

In the MODA the concepts defined in Chapter 3 and their relationships are organized in a structured collection expressing the common structure shared by all simulations: in this sense, it provides the most general way to represent a simulation with materials model(s). It contains a user case description independent of any modelling information, allowing benchmarking of different simulation and experimental approaches.

The MODA structure is composed as follows:

Table 1 — Graphical representation of the MODA structure

<table>
<tr><td colspan="2">HEADING [a]</td></tr>
<tr><td colspan="2">OVERVIEW OF THE SIMULATION [b]</td></tr>
<tr><td colspan="2">WORKFLOW [c]</td></tr>
<tr><td rowspan="4">Simulation with Model 1 [d]</td><td>1. Aspect of the user case/system to be simulated</td></tr>
<tr><td>2. Governing equations</td></tr>
<tr><td>3. Solver and computational translation of the specifications</td></tr>
<tr><td>4. Post-processing</td></tr>
<tr><td rowspan="4">Simulation with Model 2</td><td>1. Aspect of the user case/system to be simulated</td></tr>
<tr><td>2. Governing equations</td></tr>
<tr><td>3. Solver and computational translation of the specifications</td></tr>
<tr><td>4. Post-processing</td></tr>
<tr><td>...</td><td>...</td></tr>
<tr><td rowspan="4">Simulation with Model N</td><td>1. Aspect of the user case/system to be simulated</td></tr>
<tr><td>2. Governing equations</td></tr>
<tr><td>3. Solver and computational translation of the specifications</td></tr>
<tr><td>4. Post-processing</td></tr>
<tr><td colspan="2">[a] Heading, including name of the user case, project, owner
[b] Overview of the simulation, including the chain of models used
[c] Workflow, i.e. a graphical representation of the simulation
[d] Description of each part of the simulation pertaining to one model used in the chain</td></tr>
</table>

The following sections provide templates for each of the elements of the MODA.

MODA for [*user-case name*]

Simulated in project [*acronym*]

Data owner [*name, organisation, e-mail*]

Table 2 — Overview of the simulations

<table>
<tr><td colspan="4">Overview of the simulation</td></tr>
<tr><td>1</td><td>User case</td><td colspan="2">General description of the user case to be simulated (e.g. properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour).
The description shall not be longer than one sentence.
No information on modelling shall appear here.</td></tr>
<tr><td rowspan="3">2</td><td rowspan="3">Chain of models (used in the simulation)</td><td>Model 1</td><td>Physics-based model used, i.e. model name as appears in the content list of RoMM VI [1] and model type (electronic | atomistic | mesoscopic | continuum)
Data-based models can also appear here. These are described in the RoMM.</td></tr>
<tr><td>Model 2</td><td>For each model in the workflow a field shall be added here.</td></tr>
<tr><td>Model N</td><td>...</td></tr>
<tr><td>3</td><td>Publication peer-reviewing the data</td><td colspan="2">Publication documenting this particular user case and simulation approach. The publication shall ensure the quality of the calculated data (and not only the quality of the models).</td></tr>
<tr><td>4</td><td>Access conditions</td><td colspan="2">Owner and name of the software or database (include a web link if available) and whether the software and/or data are free, commercial or open source.</td></tr>
<tr><td>5</td><td>Workflow and its rationale</td><td colspan="2">Textual rationale for choosing these models and workflow instead of other possible approaches. This shall include the reason why a particular aspect of the user case is to be simulated with a particular model.</td></tr>
</table>

Table 3 — Workflow templates

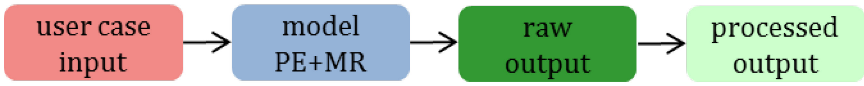
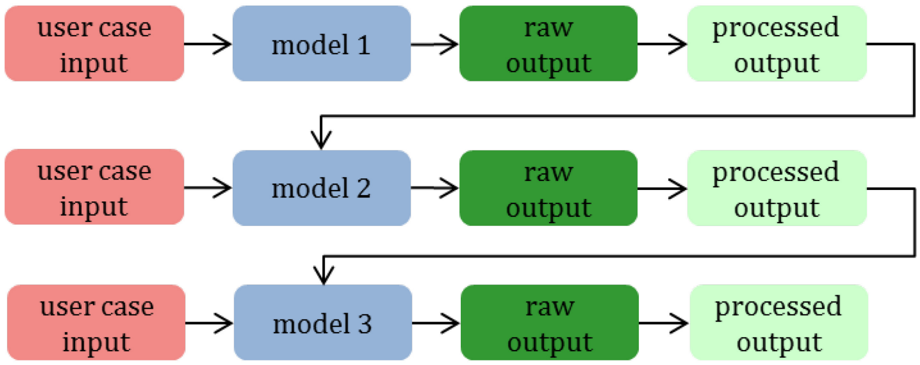
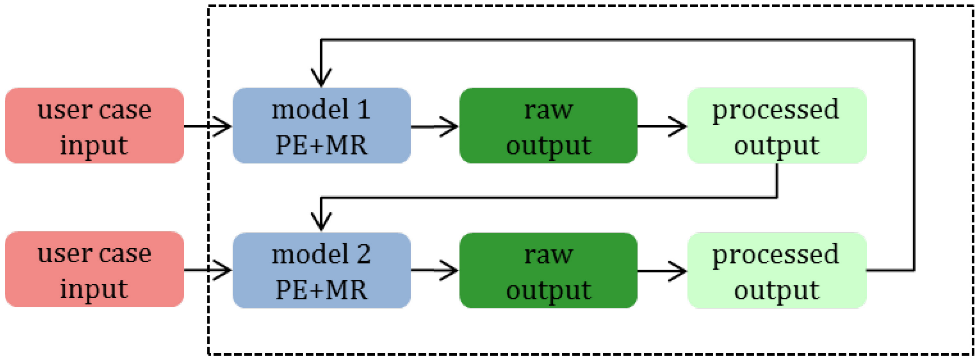
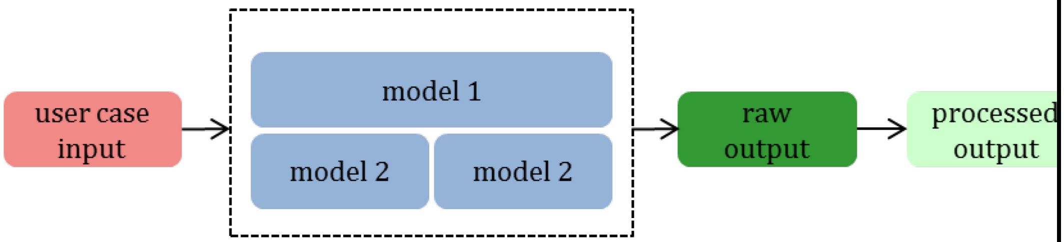
<table>
<tr><th colspan="2">Workflow templates</th></tr>
<tr><td>Workflow for a stand-alone model</td><td>
</td></tr>
<tr><td>Workflow for a chain of linked models [a]</td><td>
</td></tr>
<tr><td>Workflow for a chain of iteratively coupled models [b]</td><td>
</td></tr>
<tr><td>Workflow for tightly coupled models [c]</td><td>
</td></tr>
<tr><td colspan="2">[a] Equations solved sequentially (i. e. one-way dependency)
[b] Iterative solution of segregated equations
[c] Equations solved together (running different models for the same entity concurrently by solving one matrix)</td></tr>
</table>

Table 4 — Aspect of the user case / system to be simulated with Model n

1	Aspect of the user case / system to be simulated	
1.1	**Description of the user case aspect to be simulated with this particular model**	Textual description of the aspects of the user case to be simulated with a particular model. The information in this chapter can be end-user information, measured data, library data etc. and appears in the workflow picture as 'user case input'. They include also result of pre-processing necessary to translate the user case specifications to values for the physics parameters and variables of the entities. Simulated input which is calculated by another model shall not be included here but in 2.4. No modelling information shall appear in this box.
1.2	**Material**	Physical/chemical description of the material to be modelled.
1.3	**Geometry**	Geometry of the system to be modelled (e.g. size, form, drawing, picture of the system). This is not to be confused with the computational domain.
1.4	**Time lapse**	Duration of the situation to be simulated. This is not to be confused with the computational wall-clock time or the time step.
1.5	**Manufacturing process or in-service conditions**	Process conditions to be simulated in the model (e.g. heated walls, external pressures and bending forces). These can appear as terms in the physics equation or as boundary and initial conditions, and must be documented in the relevant chapters.
1.6	**Publication on this data**	Publication documenting the simulation with this single model and its data (if available and if not already included in the publication mentioned in the overall section).

Table 5 — Governing equations

2	Governing equations		
2.1	**Model type and name**		Model type and name chosen from RoMM content list[1]. This physics equation is represented in the blue box of the workflow picture.
2.2	**Model entity**		The entity in this physics-based model is [continuum volume | mesoscopic | atom | electron entity]
2.3	**Physics equation**	Equation	Name, description and mathematical form of the physics equation In case of tightly coupled physics equations, more than one physics equation can appear. The "raw output" calculated by the physics-based model consists per definition of values for the physics quantity variables in the physics equation(s). The raw output is depicted in the dark green box in the workflow picture.
		Physics quantities	Name of the physics quantities in the physics equation. These are parameters and variables that appear in the physics equation, like wave function, Hamiltonian, spin, velocity, external force.
2.4	**Materials relations**	Relation	Name of the materials relation and which physics equation it completes.
		Physics quantities for each materials relation	Name of the physics quantities (parameters and variables) that appear in the materials relation(s).
2.5	**Simulated input**		The information in this box documents the interoperability of the models in case of linking or iteratively coupling workflows. Simulated output of one model is input for the next model. Thus, what is entered here in 2.5 is copied from 4.1 of the model that calculated this input. For simulations in isolation this box is empty.

Table 6 — Solver and computational translation of the specification

<table>
<tr><th>3</th><th colspan="3">Solver and computational translation of the specifications</th></tr>
<tr><td>3.1</td><td>Numerical solver</td><td colspan="2">Name and type of the solver (e.g. Monte Carlo, Smoothed Particle Hydrodynamics, Finite Elements, multi-grid, adaptive)</td></tr>
<tr><td>3.2</td><td>Software tool</td><td colspan="2">Name of the code or software tool. A specification shall be added if it can be shared and a link to a website/publication can be included.</td></tr>
<tr><td>3.3</td><td>Time step</td><td colspan="2">Time step used in the solving operations. This is the numerical time step and not the time lapse of the case to be simulated (see 1.4)</td></tr>
<tr><td rowspan="3">3.4</td><td rowspan="3">Computational representation [a]</td><td>Physics equation</td><td>Computational representation of the physics equation.
Model information (physics) shall not be repeated.</td></tr>
<tr><td>Materials relations</td><td>Computational representation of the materials relation.</td></tr>
<tr><td>Material</td><td>Computational representation of the material.</td></tr>
<tr><td>3.5</td><td>Computational boundary conditions</td><td colspan="2">Translations of the physical boundary conditions set in the user case (e.g. a unit cell with periodic boundary conditions to simulate an infinite domain) or pure computational conditions</td></tr>
<tr><td>3.6</td><td>Additional solver parameters</td><td colspan="2">Pure internal numerical solver details (e.g. specific tolerances, cut-off, convergence criteria, integrator options, under relaxation parameters)</td></tr>
</table>

[a] "Computational" means that this only needs to be filled in when the solver represents the material, properties, and equation variables in a specific way.

Table 7 — Post-processing

4	Post-processing	
4.1	**The processed output**	Specification of the post-processing output. If applicable the entity in the next model shall be specified in the workflow for which this output is calculated: electrons, atoms, mesoscopic entities, larger/smaller finite volumes. This processed output appears in a light green circle in the workflow picture and also in 2.4 of the next model (if there is one). Output can be calculated values or newly established materials relations for parameters in the next physics equation.
4.2	**Methodologies**	Mathematics and/or physics used in this post-processing. In homogenisation, this is volume averaging. Not only mathematics but also physics can be used. To derive e.g. thermodynamics quantities or optical quantities from raw output of quantum mechanics models, physics equations are used that do not alter the state.
4.3	**Margin of error**	Specification of the margin of error (i.e. accuracy in percentages) of the property calculated and explanation of the reasons to an industrial end-user.

Bibliography

[1] Review of Materials Modelling: "What makes a material function? Let me compute the ways…", Anne F. de Baas (ed), 6th Version (2017), DOI: 10.2777/417118

[2] CEN Workshop Agreement CWA 16762 CEN/WS SERES - ICT Standards in Support of an eReporting Framework for the Engineering Materials Sector, May 2014 includes a definition of Material (Section A.7.2.4)