Data and documentation

*terminology, classification and ontology*

**COMMON**  terminology and classification

**EFFICIENT COMMUNICATION**

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Review of Materials Modelling
(RoMM version V and VI)


Publications, Reports
For more publications please visit the EU Bookshop

Review of Materials Modelling
(This version IV replaces the “Brochure for Materials Modelling”)

Communication between the fields will be facilitated by a commonly understood vocabulary. This vocabulary has been adapted based on extensive discussions.

The notion “meta data” has been introduced and we hope it will be used to describe models, simulation and experiment results and facilitate interoperability of different models.

We believe we have proven the vocabulary is useful by applying it to now about 100 project fishes.

Our impressions are that people have accepted the classification of models according to their physics/chemistry as the classification via application size is not unique. With this follows the separation between the notions “mesoscopic” and "mesoscale".
Standardised vocabulary and classification

**Taxonomy** CEN/CENELEC CWA


This common language can form the basis for an **ontology** with a formal language of materials modelling and a definition of the relation between the concepts.

Such an ontology can then be a basis for metadata development necessary for a Modelling Market Place.

First draft EMMO (see presentation yesterday)
MODA organise the documentation of a simulation into four tables

The tables take the modeller by the hand.
They ask the relevant questions step by step.

MODA are understandable by non–modellers.

We have proven ALL simulations can be described with this standard.

The templates and examples for the MODA standardised description can be found on (https://emmc.info/moda/)
INTRODUCTION – THE MODELLING ACTIVITY

USER CASE
material, process, phenomenon

PHYSICS MODEL
Governing Equations GE (=PE+MR).
describing the behaviour of
chosen entities
(equations for physical quantities)

NUMERICAL SOLVER
Methods and software for
the solution of
the GE (=PE+MR).

simulation

POST-PROCESSING
Extraction of results for next model
or for human-understanding.
What do we want to communicate?

- several methods (e.g. iterative solvers) and implementations (e.g. BLAS, LAPACK)

A user case can be simulated in a multitude of different ways. Choices are depending on required accuracy and limit on investments.

All situations that need to be simulated and which are experimentally measurable (i.e. everything)

User case and experimental info

Post-processing

Physics model

Numerical solver
META-MODELLING

IS IT POSSIBLE TO IDENTIFY COMMON ATTRIBUTES SHARED BY ALL MODELS?

- AB INITIO
  - Schrödinger equation
    \[ i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \left( -\frac{\hbar^2}{2\mu} \nabla^2 + V(r,t) \right) \Psi(r,t) \]

- MOLECULAR DYNAMICS
  - Newton’s law
    \[ \frac{dV}{dr} = -m \frac{d^2 r}{dt^2} \]

- COARSE GRAINED
  - Langevin equation
    \[ \langle \eta_i(t) \eta_j(t') \rangle = 2\lambda_k T \delta_{ij} \delta(t-t') \]

- CONTINUUM MODELS
  - Conservation equation
    \[ \frac{\partial \rho}{\partial t} + \nabla \cdot j = 0 \]

USER CASE

Images from
MODA (MODelling DAta)

is a template for the standardised description of materials models (https://emmc.info/moda-workflow-templates/)

The MODA is meant to guide users towards a complete high-level documentation of material models, starting from the end-user case via the computational details to the results.

It provides all necessary aspects for: description, reproducibility, curation and interfacing with other models and databases.

The MODA uses core model concepts

PHYSICS ENTITY

EQUATIONS (physics- or data-based)

a first step in the direction of a standardised description of modelling has been taken by the EC

Review of Materials Modelling VI

RoMM

Vocabulary, classification and metadata for materials modelling (130 FP7 and H2020 projects)

IN THE MODA, physics-based MATERIALS MODELS ARE CLASSIFIED VIA PHYSICS ENTITY

WHOSE BEHAVIOUR IS DESCRIBED BY PHYSICS

Bead: Discrete entity consisting of more than one atom (e.g. groups of atoms, nanoparticles, grains).

Continuum Volume: Volume in which the material properties are averaged.

The classification is
   not according to the size of the application or system
   nor according to the length scale of the phenomena to be simulated
   nor according to the solver type
PHYSICS-BASED MODEL

PHYSICS EQUATION

Equation based on a physics/chemistry theory which describes the spatial and temporal evolution of physics quantities of the entity

PE

MATERIAL RELATIONS

Information on the material needed to close the PE and to make the system of Governing Equations solvable

MR

PHYSICS QUANTITIES

EXAMPLES

CLASSICAL MOLECULAR DYNAMICS

PE

Newton's equation of motion

\[
\frac{dV}{dr} = -m \frac{d^2 r}{dt^2}
\]

MR

Lennard-Jones potential

\[
V_{LJ} = 4\epsilon \left[ \left( \frac{r}{\sigma} \right)^{12} - \left( \frac{r}{\sigma} \right)^{6} \right]
\]

FLUID DYNAMICS

PE

Navier Stokes equation

\[
\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho u \otimes u) = -\nabla \cdot p I + \nabla \cdot \sigma + \rho g
\]

Stress tensor for incompressible flows

MR

\[
\nabla \cdot \sigma = 2\mu \nabla \cdot \varepsilon = \mu \nabla \cdot (\nabla u + (\nabla u)^T) = \mu \nabla^2 u
\]
**Electronic Model**

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of electrons and quasi particles either as waves, particles or distributions.

1.1 Schrödinger Equation based models
   - Single particle Schrödinger models
   - Many body Schrödinger models
   - Quantum mechanical time dependant Schrödinger models

1.2 Kohn Sham equation Density Functional Theory (electronic DFT)

1.3 Quantum Dynamic Mean Field Theory

1.4 NEGF

1.5 Statistical charge transport model

1.6 Statistical spin transport model

**Atomistic Models**

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of atoms either as waves, particles or distributions.

2.1 Classical Density Functional Theory and Dynamic DFT

2.2 Newton's equation based models

2.3 Statistical Mechanics atomistic models

2.4 Atomistic spin models

2.5 Statistical transport model at atomistic level

2.6 Atomistic phonon-based models (Boltzmann Transport Equation)
**MESOSCOPIC MODELS**
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Beads either as waves, particles or distributions.

3.1 Mesoscopic Classical Density Functional Theory and Dynamic DFT
3.2 Coarse-Grained Molecular Dynamics and Dissipative Particle Dynamics
3.3 Statistical Mechanics mesoscopic models
3.4 Micromagnetic models
3.5 Mesoscopic phonon models (Boltzmann Transport Equation)

**CONTINUUM MODELS**
Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Continuum Volume.

4.1 Solid Mechanics
4.2 Fluid Mechanics
4.3 Heat Flow and Thermo-mechanical behaviour
4.4 Continuum Thermodynamics and Phase Field models
4.5 Chemistry reaction (kinetic) models (continuum)
4.6 Electromagnetism (incl optics, magnetics and electrical)

Processes and Devices
MODA – TEMPLATE SNAPSHOTS

HOW IT LOOKS!

USER CASE

1. General description of the User Case
   - Please give the properties and behavior of the particular material, data, dataflow, and/or other environment to be simulated.
   - Information on the simulation model should appear here.

2. OVERVIEW OF THE SIMULATION
   - General overview of the simulation.

3. CRASH OF MODEL
   - Identify the first model. If you are unsure, please specify.
   - All data-driven models used, please specify.

4. POST-PROCESSING
   - Please specify the output, data, and/or results.
   - Post-processing outputs may include:
     - Simulation data
     - Plots and graphs
     - Reports and summaries

5. PROGRAMMING LANGUAGES
   - Please specify the programming language used.
   - Examples include:
     - MATLAB
     - Python
     - C++

6. ADDITIONAL COMMENTS
   - Additional comments or notes.

MODEL PHYSICS OF THE MODEL EQUATION

1. General model
   - This model is used to describe the behavior of the system.
   - The model is based on the physical laws governing the system.
   - The model is defined by a set of differential equations.

2. PHYSICAL QUANTITIES
   - Physical quantities are the variables that describe the physical system.
   - Examples include:
     - Temperature
     - Pressure
     - Velocity

3. MATHEMATICAL RELATION
   - Mathematical equations that describe the behavior of the system.
   - Examples include:
     - Continuity equation
     - Momentum equation
     - Energy equation

4. SIMULATION SETUP
   - Please specify the simulation setup.
   - Examples include:
     - Boundary conditions
     - Initial conditions
     - Time step

5. POST-PROCESSING
   - Please specify the output, data, and/or results.
   - Post-processing outputs may include:
     - Simulation data
     - Plots and graphs
     - Reports and summaries

6. ADDITIONAL COMMENTS
   - Additional comments or notes.

ECOLOGY AND COMPUTATIONAL SIMULATION OF THE SPECIFICATIONS

1. SPECIFICATIONS
   - Please give the specifications of the user case.
   - Examples include:
     - Number of elements
     - Mesh size
     - Time step

2. SOFTWARE TOOLS
   - Please give the names of the software tools used.
   - Examples include:
     - ANSYS
     - COMSOL
     - MATLAB

3. TIME STEP
   - Please give the time step used in the simulation.
   - Examples include:
     - Fixed time step
     - Adaptive time step

4. COMPUTATIONAL REPRESENTATION
   - Please give the computational representation of the model.
   - Examples include:
     - Finite element method
     - Finite difference method
     - Boundary element method

5. COMPUTATIONAL ELEMENTS
   - Please give the computational elements used.
   - Examples include:
     - Tetrahedral elements
     - Hexahedral elements
     - Triangular elements

6. ADDITIONAL COMMENTS
   - Please give additional comments or notes.
   - Examples include:
     - Methodology
     - Validation
     - Verification

POST-PROCESSING

1. POST-PROCESSING SETUP
   - Please specify the post-processing setup.
   - Examples include:
     - Data visualization
     - Animation
     - Reports

2. RESULTS ANALYSIS
   - Please specify the results analysis.
   - Examples include:
     - Statistical analysis
     - Graphical analysis
     - Comparison with experimental data

3. ADDITIONAL COMMENTS
   - Please give additional comments or notes.
   - Examples include:
     - Conclusion
     - Limitations
     - Future work
MODA – TEMPLATE STRUCTURE

OVERVIEW OF THE SIMULATION

MODEL 1

User Case

Model Physics

Solver

Post Processing

MODEL 2

User Case

Model Physics

Solver

Post Processing

...  

MODEL n

Linked WORKFLOW

user case input

to

model 1

to raw output

to processed output

user case input

to

model 2

to raw output

to processed output

user case input

to

model 3

to raw output

to processed output
MODA WORKFLOW

workflow for an iterative chain

Iterative solution of segregated equations

workflow for tightly coupled models

equations solved together
(running different models for the same entity concurrently by solving one matrix)
# OVERVIEW of the SIMULATION

**USER CASE**

General description of the User Case: **properties** and **behaviour** of the particular **material**, **manufacturing process** and/or **in-service-behaviour** to be simulated.

**No information on the modelling** should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.

**CHAIN OF MODELS**

<table>
<thead>
<tr>
<th>MODEL 1</th>
<th>Please identify all models used in this simulation. Note these are assumed to be physics-based models unless it is specified differently.</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODEL 2</td>
<td>Most modelling projects consist of a chain of models (workflow). Only names appearing in the content list of the Review of Materials Modelling VI should be entered. All models should be identified as electronic, atomistic, mesoscopic or continuum.</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
<tr>
<td>MODEL N</td>
<td></td>
</tr>
</tbody>
</table>

**DATA-BASED MODEL**

If data-based models are used, please specify.

**PUBLICATION PEER-REVIEWING THE DATA**

The publication which documents the data of this ONE simulation.

This article should ensure the quality of this data set (and not only the quality of the models).

**ACCESS CONDITIONS**

List whether the model and/or data are **free**, **commercial** or **open source** and the **owner** and the name of the software or database (include a web link if available).

**WORKFLOW AND ITS RATIONALE**

Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently. Please discuss the balance between wished for accuracy (of properties or trend predictions) and necessary investment.

This should include the reason why a particular aspect of the user case is to be simulated with a particular model.
# Aspects of the User Case to be Simulated

<table>
<thead>
<tr>
<th>Model 1, 2, ..., N (one for each model in the chain)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aspect of the User Case to be Simulated</strong></td>
</tr>
<tr>
<td><strong>Material</strong></td>
</tr>
<tr>
<td><strong>Description</strong> of the material to be simulated (e.g. chemical composition)</td>
</tr>
<tr>
<td><strong>Geometry</strong></td>
</tr>
<tr>
<td><strong>Size, form, picture of the system</strong> (if applicable)</td>
</tr>
<tr>
<td><strong>Time Lapse</strong></td>
</tr>
<tr>
<td><strong>Duration</strong> of the User Case to be simulated.</td>
</tr>
<tr>
<td>This is the duration of the <strong>situation to be simulated</strong>. This is not the same as the computational times.</td>
</tr>
<tr>
<td><strong>Manufacturing Process or In-service Conditions</strong></td>
</tr>
<tr>
<td>If relevant, please list the <strong>conditions to be simulated</strong> (if applicable).</td>
</tr>
<tr>
<td>e.g. heated walls, external pressures and bending forces. Please note that these might appear as terms in the PE or as boundary and initial conditions, and this will be documented in the relevant chapters</td>
</tr>
<tr>
<td><strong>Publications on this Data</strong></td>
</tr>
<tr>
<td>Publication <strong>documenting the simulation</strong> with this single model and its data (if available and if not already included in the overall publication).</td>
</tr>
</tbody>
</table>

**Describe the aspects of the User Case textually.**

**No modelling information** should appear in this box. This case could also be simulated by other models in a benchmarking operation!

The information in this chapter can be **end-user information, measured data, library data** etc. It will appear in the pink circle of your workflow picture.

**Simulated input** which is calculated by another model should not be included.

Also the result of **pre-processing** necessary to translate the user case specifications to values for the physics variables of the entities can be documented here.
# MODA – Generic Physics of the Model Equation

| MODEL TYPE AND NAME | Model type and name *chosen from RoMM content list.*  
| This PE and only this will appear in the blue circle of your workflow picture. |
| MODEL ENTITY | The *entity* in this materials model is `<finite volumes, beads, atoms, or electrons>` |
| MODEL PHYSICS EQUATIONS | **EQUATION**  
| Name, description and mathematical form of the PE  
In case of tightly coupled PEs set up as one matrix which is solved in one go, more than one PE can appear. |
| PHYSICAL QUANTITIES | Please name the *physics quantities in the PE*, these are parameters (constants, matrices) and variables that appear in the PE, like wave function, Hamiltonian, spin, velocity, external force. |
| MATERIAL RELATIONS | **RELATION**  
Please, give the name of the *Material Relation* and which PE it completes. |
| PHYSICAL QUANTITIES | Please give the name of the *physics quantities*, parameters (constants, matrices) and variables that appear in the MR(s) |

## Simulated Input

*Please document the *simulated input* and with which model it is calculated.  
This box documents the *interoperability of the models in case of sequential or iterative model workflows*. Simulated output of the one model is input for the next model. Thus what you enter here will also appear as processed output of the model that calculated this input.  
*If you do simulations in isolation*, then this box will *remain empty*. |
<table>
<thead>
<tr>
<th>MODEL 1, 2, ..., N (one for each model in the chain)</th>
<th><strong>SOLVER AND TRANSLATION OF THE SPECIFICATIONS</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NUMERICAL SOLVER</strong></td>
<td>Please give <strong>name</strong> and <strong>type</strong> of the solver.</td>
</tr>
<tr>
<td></td>
<td>e.g. Monte Carlo, SPH, FE, iterative, multi-grid, adaptive,...</td>
</tr>
<tr>
<td><strong>SOFTWARE TOOL</strong></td>
<td>Please give the <strong>name of the code</strong> and if this is your own code, please specify if it can be shared with an eventual link to a website/publication.</td>
</tr>
<tr>
<td><strong>TIME STEP</strong></td>
<td>If applicable, please give the <strong>time step</strong> used in the solving operations.</td>
</tr>
<tr>
<td></td>
<td>This is the <strong>numerical time step</strong> and this is not the same as the time lapse of the case to be simulated.</td>
</tr>
<tr>
<td><strong>COMPUTATIONAL REPRESENTATION</strong></td>
<td><strong>PHYSICS EQUATION</strong></td>
</tr>
<tr>
<td></td>
<td>Computational representation of the Physics Equation, Materials Relation and material.</td>
</tr>
<tr>
<td></td>
<td><strong>MATERIAL RELATIONS</strong></td>
</tr>
<tr>
<td></td>
<td>There is no need to repeat User Case info. “Computational” means that this only needs to be filled in when your computational solver represents the material, properties, equation variables, in a specific way.</td>
</tr>
<tr>
<td></td>
<td><strong>MATERIAL</strong></td>
</tr>
<tr>
<td><strong>COMPUTATIONAL BOUNDARY CONDITIONS</strong></td>
<td>Please note that these can be translations of the <strong>physical boundary conditions</strong> set in the User Case or they can be pure <strong>computational</strong> like e.g. a unit cell with mirror boundary conditions to simulate an infinite domain.</td>
</tr>
<tr>
<td><strong>ADDITIONAL SOLVER PARAMETERS</strong></td>
<td>Please specify <strong>pure internal numerical solver details</strong> (if applicable), like specific tolerances, cut-off, convergence criteria.</td>
</tr>
<tr>
<td>MODEL 1, 2, ..., N (one for each model in the chain)</td>
<td>POST PROCESSING</td>
</tr>
<tr>
<td>--------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td><strong>THE PROCESSED OUTPUT</strong></td>
<td>The output obtained by the post processing (e.g. values for parameters, new MR and descriptor rules for data-based models). Specify the entity in the next model in the chain for which this output is calculated: electrons, atoms, beads (e.g. nanoparticles, grains), volume elements. In case of homogenisation, please specify the averaging volumes.</td>
</tr>
<tr>
<td><strong>METHODOLOGIES</strong></td>
<td>Please describe the mathematics and/or physics used in this post-processing calculation (e.g. volume averaging, physical relations for thermodynamics quantities or optical quantities calculation)</td>
</tr>
<tr>
<td><strong>MARGIN OF ERROR</strong></td>
<td>Please specify the accuracy in percentages of the property calculated and explain the reasons to an industrial end-user.</td>
</tr>
</tbody>
</table>
Models based on extraction/identification of relations between descriptors using data-mining on simulated or experimental data.

They are best-fitting, phenomenological models. They are often called surrogate models in engineering.

These simplified relations when used in isolation do not always need complicated numerical solvers as they are able to find quick answers.

We will collectively call these relations data-based models. The database from which these relations are extracted should always be documented.
ELASTIC PROPERTIES OF A POLYCRYSTALLINE POLYPROPYLENES

- **Process conditions**
- **Thermodynamic data**
- **Arrangement of atoms, temperature, Interatomic potentials**

**Tightly coupled continuum models**
- Multiphase flow model (CFD) coupled with heat and flow front equations
- Thermodynamic based model for nucleation and growth
- Molecular Dynamics

**Microstructure**
- Temperature, flow velocity phase fractions
- Microstructure: spherulites, fraction amorp., centroids of spherulites, additional interfaces

**Experimental geometry of a bilamella**
- Conditions at location of single RVE
- Microstructure, effective, anisotropic thermomechanical properties of injection moulded polypropylene microstructures

**Two level homogenisation procedure**
- Mechanical properties of isotactic PP crystalline phase
Functioning & stability-limiting mechanisms organic phosphorescent OLEDs

**Electronic model**
- **Model 1**
  - GW, BSE
  - ~ 10^2 atoms
  - Relaxed geometries Wave functions Eigenenergies
  - Polarizable force fields Excitation DOS’s Reorganization energies Transfer Integrals

- **Model 2**
  - MD
  - ~ 10^4 - 10^5 atoms
  - Atomic positions
  - Amorphous morphology Electrostatic & polarization contribution to site energies

**Mesoscopic model**
- **Model 3**
  - BTE
  - ~ 10^6 - 10^7 sites
  - Time-dependent positions and distributions of quasiparticles
  - Charge mobilities Exciton diffusion coefficients Recombination & generation rates Exciton decay rates Charge-exciton & exciton-exciton quenching rates

**Continuum model**
- **Model 4**
  - DD
  - Time-dependent distributions of quasiparticles
  - Current- & luminescence-voltage characteristics Luminescence efficiency & roll-off Emission profile & colour balance Degradation rate
Density Functional Theory

Bulk & surface structure
Mechanisms Catalytic Reactions

Electronic model
Density Functional Theory

Wavefunctions
Energies

COHP, DOS, Bader etc
Bonding trends
Dominant catalytic surfaces

Transition state
Eyring equation
Stat TD
Rate Parameters

Overall reaction rates,
selectivity, optimum
particle size
Reaction rates
Limitations in process
(descriptor based rules)

Partial PGMs

law of mass action
& CFD

KMC
Particle positions
Coverage rates

Tightly coupled
continuum models
Law of Mass Action & CFD

Mesoscopic model

user case input
model
raw output
processed output
**Metadata** are defined as data and schema that describe and give information about a data describing a specific domain knowledge.

**MODA as top-level METADATA SCHEMA**

- **exchange of information** between materials modelling models (can also be in the same code)
- putting data in a form that allows modellers to **recognise** them along with their meaning.
- deal with the complexity of **sharing data between multiple tools** (in-house and commercial; proprietary and open)
- **code generation** (meta-programming of classes and structures)
• Develop MODA online form for easy compilation, catalogue and formatting.
  • Distinguish between free text field entries (e.g. description) and fixed options (e.g. model entities)
  • Provide standard PE for the 24 model types so that every applicant will not need to reinvent the wheel
  • Provide a first set of standard MR for the most common models

• Provide a navigable selected set of MODA examples (from RoMM VI) for different fields of applications to be used as reference point

• Develop formal taxonomy and ontology
YOU CAN FIND ALL THESE THINGS EXTENSIVELY EXPLAINED IN THE RoMM VI

THANKS FOR YOUR ATTENTION

Review of Materials Modelling VI RoMM

Edited by Anne F de Baas

Vocabulary, classification and metadata for materials modelling (130 FP7 and H2020 projects)


Short version of RoMM VI