RoMM VI

towards Digital Single Market

MATERIALS MODELLING

EMMC

Data and documentation
terminology, classification and ontology

COMMON terminology and classification

EFFICIENT COMMUNICATION

Dr. Anne F de Baas, EC

November 2017

Review of Materials Modelling (RoMM version V and VI)

http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

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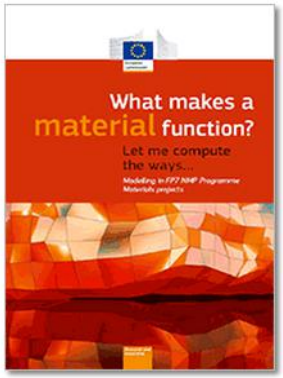
Review of Materials Modelling

(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 fiches.

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".

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Review of Materials Modelling (RoMM version V and VI)

Standardised vocabulary and classification
Taxonomy CEN/CENELEC CWA
https://www.cen.eu/news/workshops/Pages/WS-2017-012.aspx .

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 a unified presentation

MODA organise the documentation of a simulation into four tables

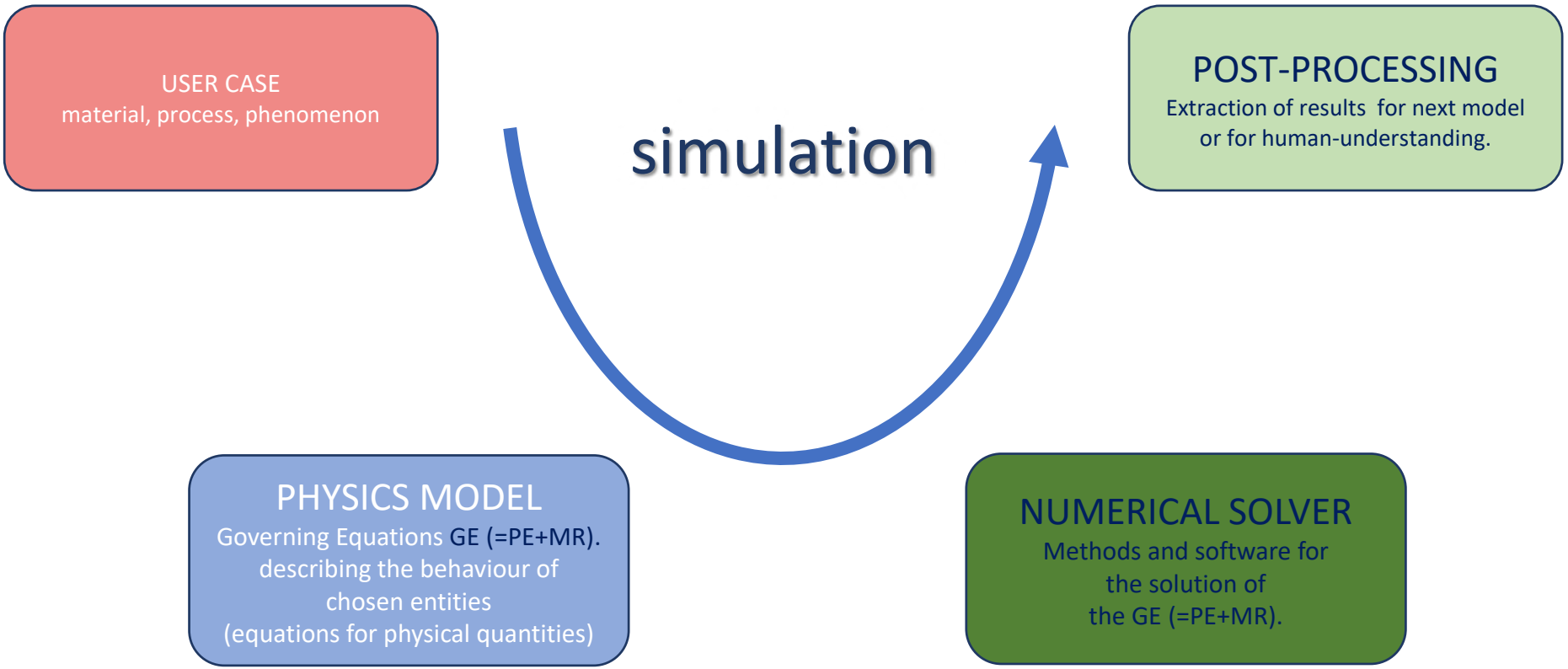
The tables take the modeller by the hand.
They ask the relevant questions step by step.

MODA are understandable by non –modellers.

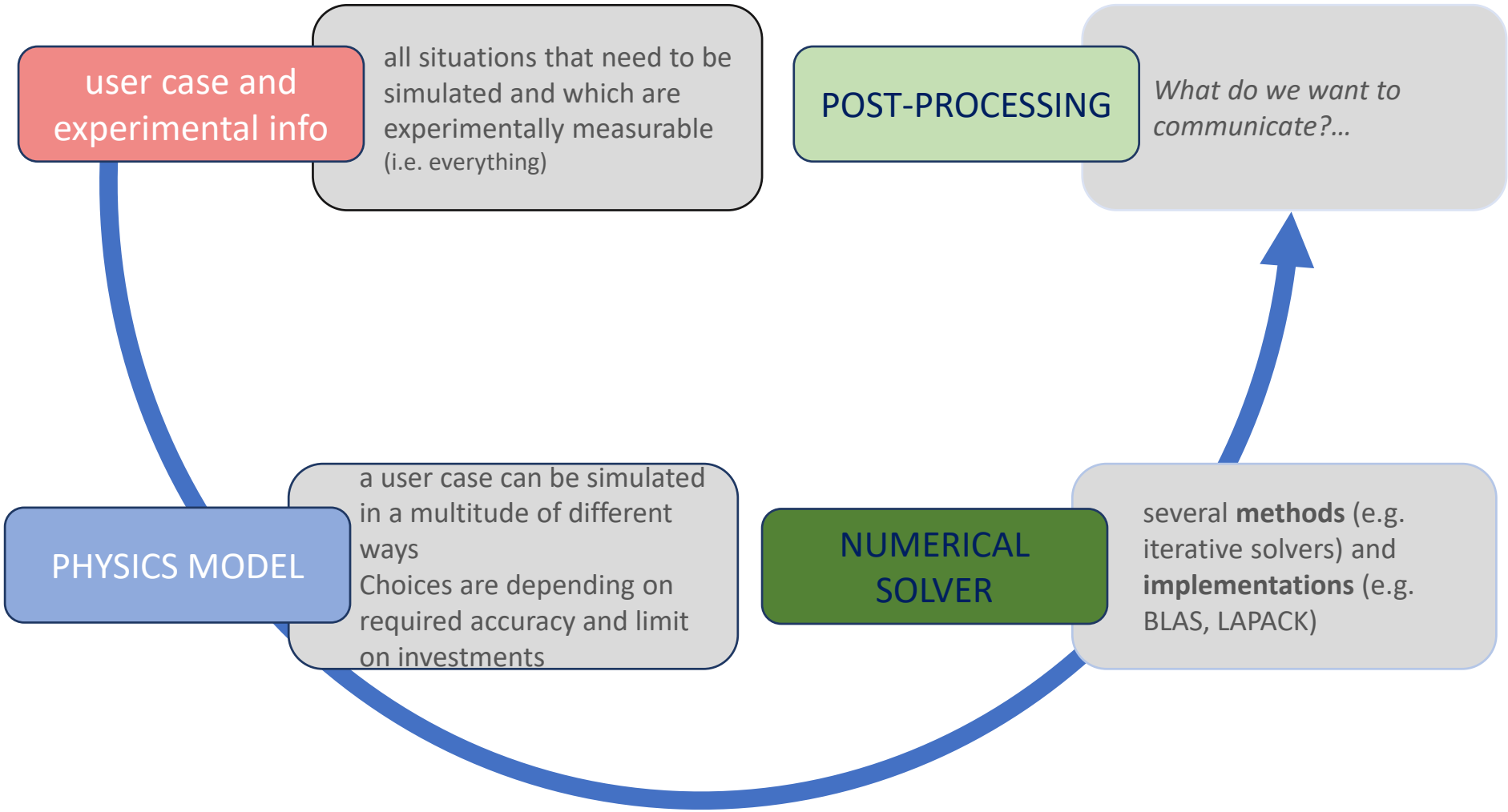
We have proven ALL simulations can be described with this standard.

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

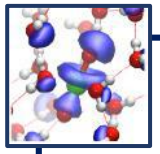
INTRODUCTION – THE MODELLING ACTIVITY



HOW TO COLLAPSE A COMPLEX WORLD ONTO A SIMPLE SYSTEM



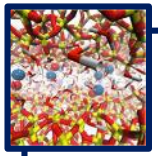
IS IT POSSIBLE TO IDENTIFY
COMMON ATTRIBUTES
SHARED BY ALL MODELS?



AB INITIO

Schrödinger equation

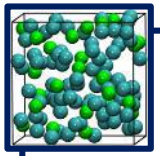
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$



MOLECULAR DYNAMICS

Newton's law

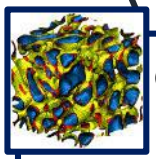
$$\frac{dV}{dr} = -m\frac{d^2r}{dt^2}$$



COARSE GRAINED

Langevin equation

$$\langle \eta_i(t)\,\eta_j(t')\rangle = 2\lambda k_B T \delta_{i,j}\delta(t-t').$$



CONTINUUM MODELS

Conservation equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

USER CASE

Images from

MODA DEFINITION

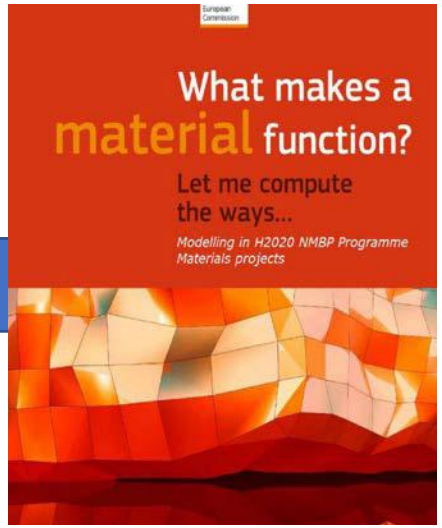
a first step in the direction of a standardised description of modelling has been taken by the EC

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.



Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology projects

Review of Materials Modelling VI
RoMM

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

https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/

The MODA uses **core model concepts**

PHYSICS ENTITY

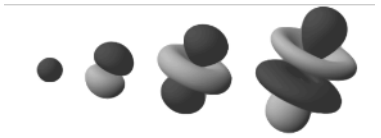
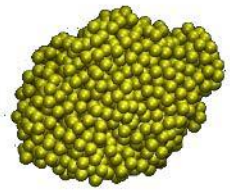
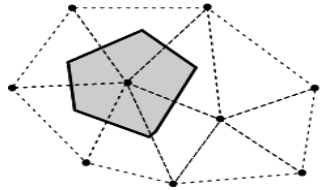
EQUATIONS (physics- or data-based)

MODA – MODEL ENTITIES

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

PHYSICS ENTITY → Self-contained, physically distinct, internally frozen, physical 'object'

WHOSE BEHAVIOUR IS DESCRIBED BY PHYSICS

ELECTRONS	ATOMS	BEADS	CONTINUUM VOLUME
			

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**

MODA – Physics-based Model Definition

PHYSICS-BASED MODEL

PHYSICS EQUATION
PE

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

PHYSICS QUANTITIES

MATERIAL RELATIONS
MR

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

EXAMPLES

CLASSICAL MOLECULAR DYNAMICS

PE
Newton's equation of motion

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

MR
Lennard-Jones potential

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

FLUID DYNAMICS

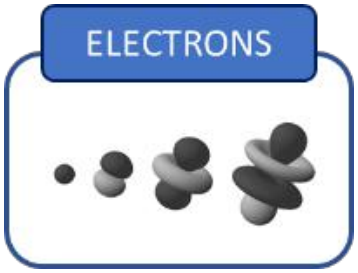
PE
Navier Stokes equation

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla\cdot p\mathbf{I} + \nabla\cdot\boldsymbol{\tau} + \rho\mathbf{g}$$

MR
Stress tensor for incompressible flows

$$\nabla\cdot\boldsymbol{\tau} = 2\mu\nabla\cdot\boldsymbol{\varepsilon} = \mu\nabla\cdot\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right) = \mu\nabla^2\mathbf{u}$$

MODA – 24 Model Types

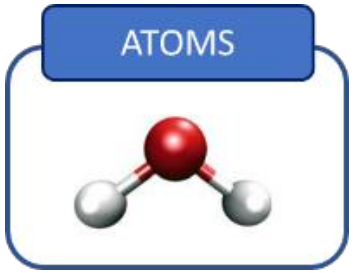


Electronic Model

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

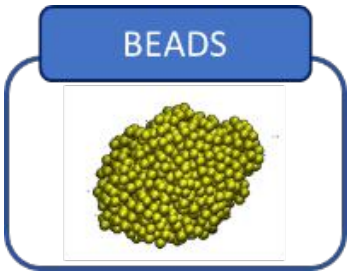


Atomistic Models

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)

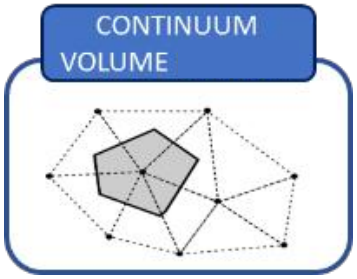
MODA – 24 PHYSICS-BASED MODEL TYPES



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

HOW IT LOOKS!

MODA for <user-case>
***Simulated* in project <acronym>**

OVERVIEW of the SIMULATION			
1	User Case		*General description of the User Case.* *Please give the 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.*
2	Chain of Models	Model 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm) All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		Model 2	*Please identify the second model.*
		Data-based model	*If data-based models are used, please specify.*
3	Publication Peer-Reviewing the data		*Please give 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).*
4	Access conditions		*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*
5	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.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

1	Aspect of the User Case/System to be Simulated	
1.1	Aspect of the User Case to be simulated	*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 (but this input is listed in chapter 2.4)* *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.*
1.2	Material	*Chemical composition, ...*
1.3	Geometry	*Size, form, picture of the system (if applicable)* *Note that computational choices like simulation boxes are to be documented in chapter 3.*
1.4	Time Lapse	*Duration of the User Case to be simulated.* *This is the duration of the situation to be simulated. This is not the same as the computational times to be given in chapter 3.*
1.5	Manufacturing process or in-service conditions	*If relevant, please list the conditions to be simulated (if applicable).* *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.*
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 overall publication).*

2	Generic Physics Of The Model Equation		
2.0	Model type and name		*Model type and name **chosen from RoMM content list** (the PE).* *This PE and only this will appear in the blue circle of your workflow picture. Please do not insert any other text although an indication of the MR is allowed.*
2.1	Model entity		*The entity in this materials model is <finite volumes, grains, atoms, or electrons>*
2.2	Model Physics/ Chemistry equation PE	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.*
		Relation	*Please, give the name of the Material Relation and which PE it completes.*
2.3	Materials relations	Physical quantities/ descriptors for each MR	*Please give the name of the physics quantities, parameters (constants, matrices) and variables that appear in the MR(s)*
2.4	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 in 2.4 will also appear in 4.1 of the model that calculated this input.* *If you do simulations in isolation, then this box will remain empty.* *Note that all measured input is documented in chapter 1 "User Case".*

3	Solver and Computational translation of the specifications		
3.1	Numerical Solver		*Please give name and type of the solver. E.g. Monte Carlo, SPH, FE, ...iterative, multi-grid, adaptive,...*
3.2	Software tool		*Please give the name of the code and if this is your own code, please specify if it can be shared with an eventual link to a website/publication.*
3.3	Time step		*If applicable, please give the time step used in the solving operations. This is the numerical time step and this is not the same as the time lapse of the case to be simulated (see 1.4)*
3.4	Computational Representation	Physics Equation, Material Relations, Material	*Computational representation of the Physics Equation, Materials Relation and material.* *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.*
3.5	Computational boundary conditions		*If applicable.* *Please note that these can be translations of the physical boundary conditions set in the User Case or they can be pure computational like e.g. a unit cell with mirror b.c. to simulate an infinite domain.*
3.6	additional Solver Parameters		*Please specify pure internal numerical solver details (if applicable), like* • *specific tolerances,* • *cut-off, convergence criteria* • *integrator options*

4	POST PROCESSING	
4.1	The processed output	*Please specify the output obtained by the post processing.* *If applicable then specify the entity in the next model in the chain for which this output is calculated: electrons, atoms, grains, larger/smaller finite volumes.* *In case of homogenisation, please specify the averaging volumes.* *Output can be calculated values for parameters, new MR and descriptor rules (data-based models).*
4.2	Methodologies	*Please describe the mathematics and/or physics used in this post-processing calculation.* *In homogenisation this is volume averaging. But also physics equations can be used to derive e.g. thermodynamics quantities or optical quantities from Quantum Mechanics raw output.*
4.3	Margin Of Error	*Please specify the margin of error (accuracy in percentages) of the property calculated and explain the reasons to an industrial end-user.*

MODA – TEMPLATE STRUCTURE

OVERVIEW OF THE SIMULATION

MODEL 1

- User Case
- Model Physics
- Solver
- Post Processing

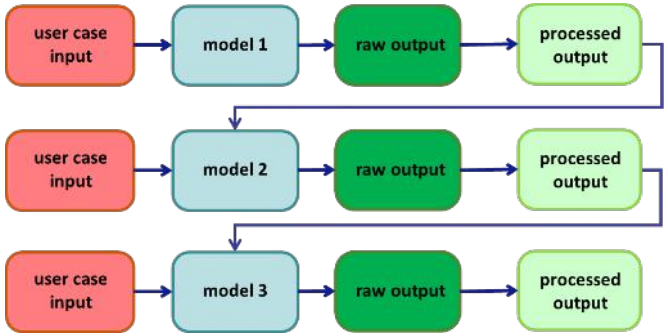
MODEL 2

- User Case
- Model Physics
- Solver
- Post Processing

...

MODEL n

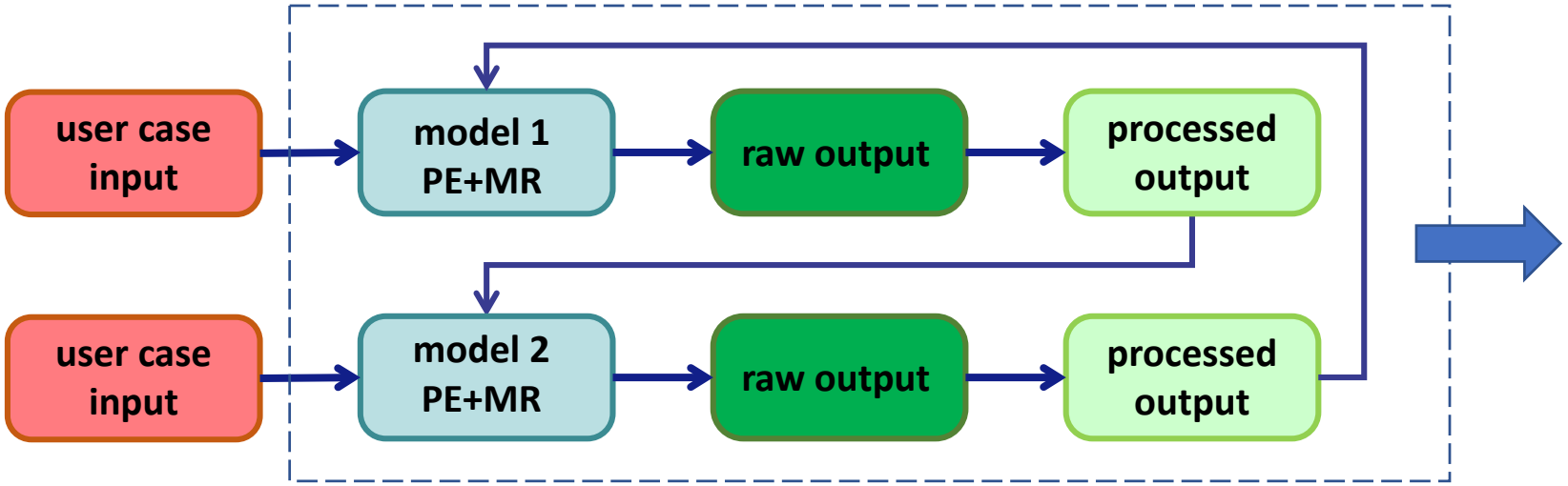
Linked WORKFLOW



MODA Workflow

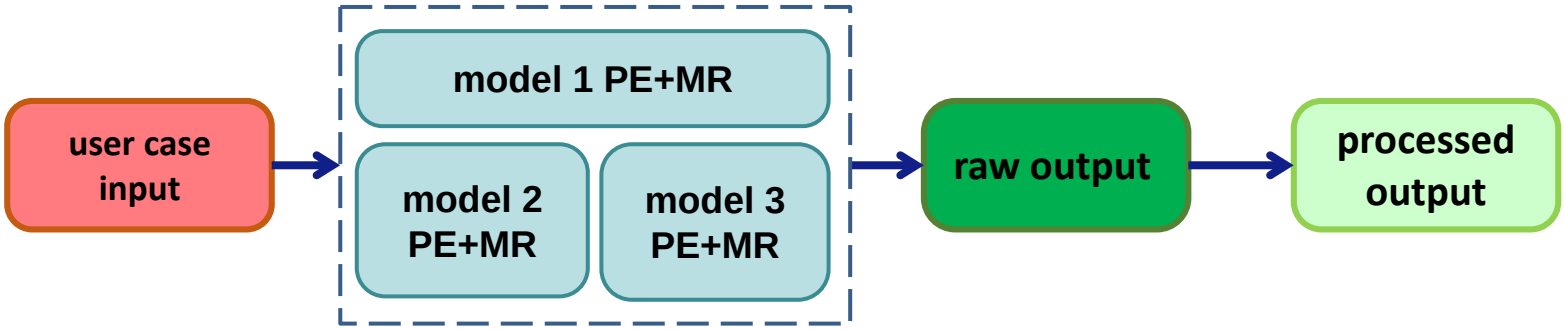
workflow for an iterative chain

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)



MODA – Overview Of The Simulation

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	**Model 1**	*Please identify **all models used in this simulation**. Note these are assumed to be physics-based models unless it is specified differently.* *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**.*
	Model 2	
	…	
	Model N	
	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.*	

MODA – Physics-based Model: Aspect of the User Case

MODEL 1, 2, …, N *(one for each model in the chain)*	Aspect of the User Case to be Simulated	
	Aspect of the User Case to be Simulated	*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.*
	Material	***Description** of the material to be simulated (e.g. chemical composition)*
	Geometry	***Size**, **form**, **picture of the system** (if applicable)*
	Time Lapse	***Duration** of the User Case to be simulated.* *This is the duration of the **situation to be simulated**. This is not the same as the computational times.*
	Manufacturing process or In-service conditions	*If relevant, please list the **conditions to be simulated** (if applicable).* *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*
	Publications on this data	*Publication **documenting the simulation** with this single model and its data (if available and if not already included in the overall publication).*

MODA – Generic Physics of the Model Equation

MODEL 1, 2, …, N *(one for each model in the chain)*

Model Equations		
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**.*	

MODA – Solver and Computational Translation

MODEL 1, 2, …, N *(one for each model in the chain)*

Solver and Translation of the Specifications		
Numerical Solver	*Please give **name** and **type** of the solver.* *e.g. Monte Carlo, SPH, FE, iterative, multi-grid, adaptive,…*	
Software Tool	*Please give the **name of the code** and if this is your own code, please specify if it can be shared with an eventual link to a website/publication.*	
Time Step	*If applicable, please give the **time step** used in the solving operations.* *This is the **numerical time step** and this is not the same as the time lapse of the case to be simulated.*	
Computational Representation	**Physics Equation**	*Computational representation of the Physics Equation, Materials Relation and material.* *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.*
	Material Relations	
	Material	
Computational Boundary Conditions	*Please note that these can be translations of the **physical boundary conditions** set in the User Case or they can be pure **computational** like e.g. a unit cell with mirror boundary conditions to simulate an infinite domain.*	
Additional Solver Parameters	*Please specify **pure internal numerical solver details** (if applicable), like specific tolerances, cut-off, convergence criteria.*	

MODA – POST PROCESSING

MODEL 1, 2, …, N *(one for each model in the chain)*	POST PROCESSING	
	THE PROCESSED OUTPUT	*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.*
	METHODOLOGIES	*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)*
	MARGIN OF ERROR	*Please specify the **accuracy in percentages** of the property calculated and **explain the reasons to an industrial end-user**.*

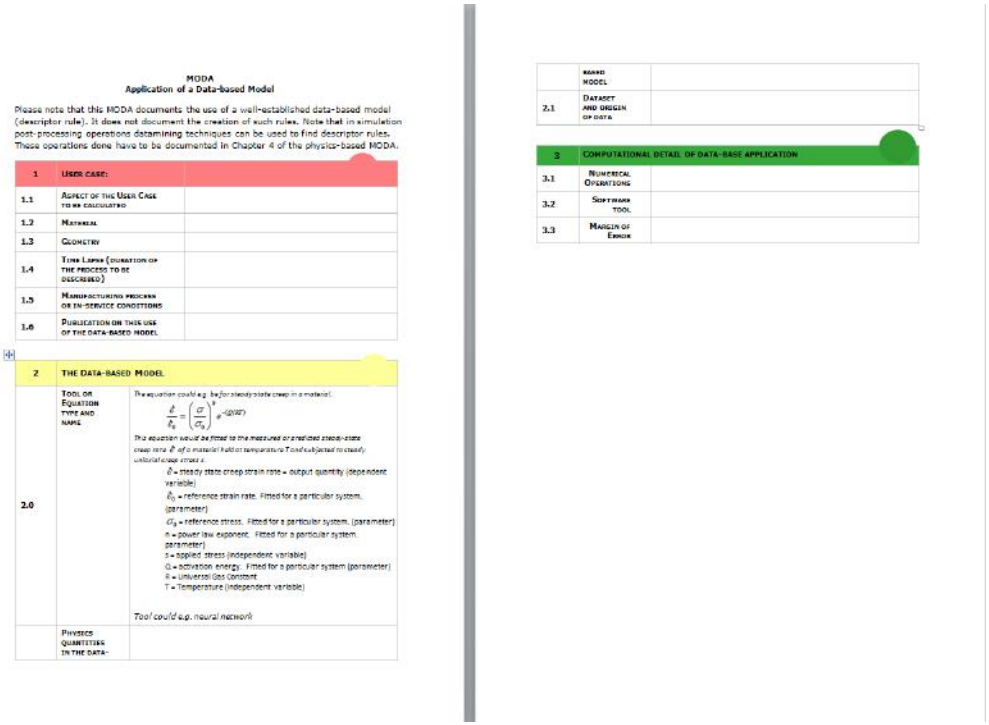
MODA – Data-Based Model

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.



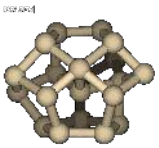
MODA
Application of a Data-based Model

Please note that this MODA documents the use of a well-established data-based model (descriptor rule). It does not document the creation of such rules. Note that in simulation post-processing operations datamining techniques can be used to find descriptor rules. These operations done have to be documented in Chapter 4 of the physics-based MODA.

1	USER CASE:	
1.1	ASPECT OF THE USER CASE TO BE CALCULATED	
1.2	MATERIAL	
1.3	GEOMETRY	
1.4	TIME LAPSE (DURATION OF THE PROCESS TO BE DESCRIBED)	
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	
1.6	PUBLICATION ON THIS USE OF THE DATA-BASED MODEL	
2	THE DATA-BASED MODEL	
2.0	TOOL OR EQUATION TYPE AND NAME	The equation could e.g. be for steady state creep in a material: $\frac{\dot{\delta}}{\dot{\delta}_0} = \left(\frac{\sigma}{\sigma_0}\right)^n e^{-\left(\frac{Q}{RT}\right)}$ This equation would be fitted to the measured or predicted steady-state creep rate $\dot{\delta}$ of a material held at temperature T and subjected to steady uniaxial creep stress σ. $\dot{\delta}$ = steady state creep strain rate = output quantity (dependent variable) $\dot{\delta}_0$ = reference strain rate. Fitted for a particular system. (parameter) σ_0 = reference stress. Fitted for a particular system. (parameter) n = power law exponent. Fitted for a particular system. parameter) σ = applied stress (independent variable) Q = activation energy. Fitted for a particular system (parameter) R = Universal Gas Constant T = Temperature (independent variable) *Tool could e.g. neural network*
	PHYSICS QUANTITIES IN THE DATA-	
	BASED MODEL	
2.1	DATASET AND ORIGIN OF DATA	
3	COMPUTATIONAL DETAIL OF DATA-BASE APPLICATION	
3.1	NUMERICAL OPERATIONS	
3.2	SOFTWARE TOOL	
3.3	MARGIN OF ERROR	

USE CASE

NanoDome



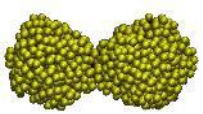
ELECTRONIC MODEL

Atomic species N<50

QUANTUM MECHANICS (eDFT)

Wavefunction, Energies

– Cluster of atoms (e.g. structure, bonds, radial distribution function)
– ReaxFF parameters



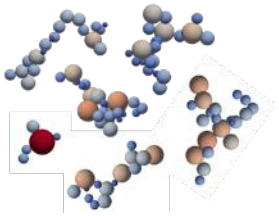
ATOMISTIC MODEL

Atomic species N>50

CLASSICAL MOLECULAR DYNAMICS (ReaxFF potential)

Atomic system evolution in time (i.e. nanoparticle formation)

– Nucleation rates
– Surface reaction rates
– Inter-nanoparticle forces



– Pressure
– Temperature
– Species concentrations

OR

MESOSCOPIC MODEL

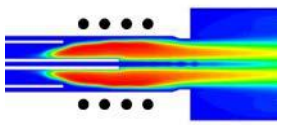
LANGEVIN MOTION

FRIEDLANDER-KOCH SINTERING EQUATION

DIFFUSION-REACTION EQUATION

Nanoparticle system evolution in time (i.e. growth, aggregation, agglomeration, sintering)

– Particle size distribution
– Chemical composition
– Vapour consumption



Process operating conditions (e.g. reactor type and geometry, power, precursor feed rate, process gas)

CONTINUUM MODEL

TRANSPORT EQUATION (mass, momentum, energy)

TURBULENCE

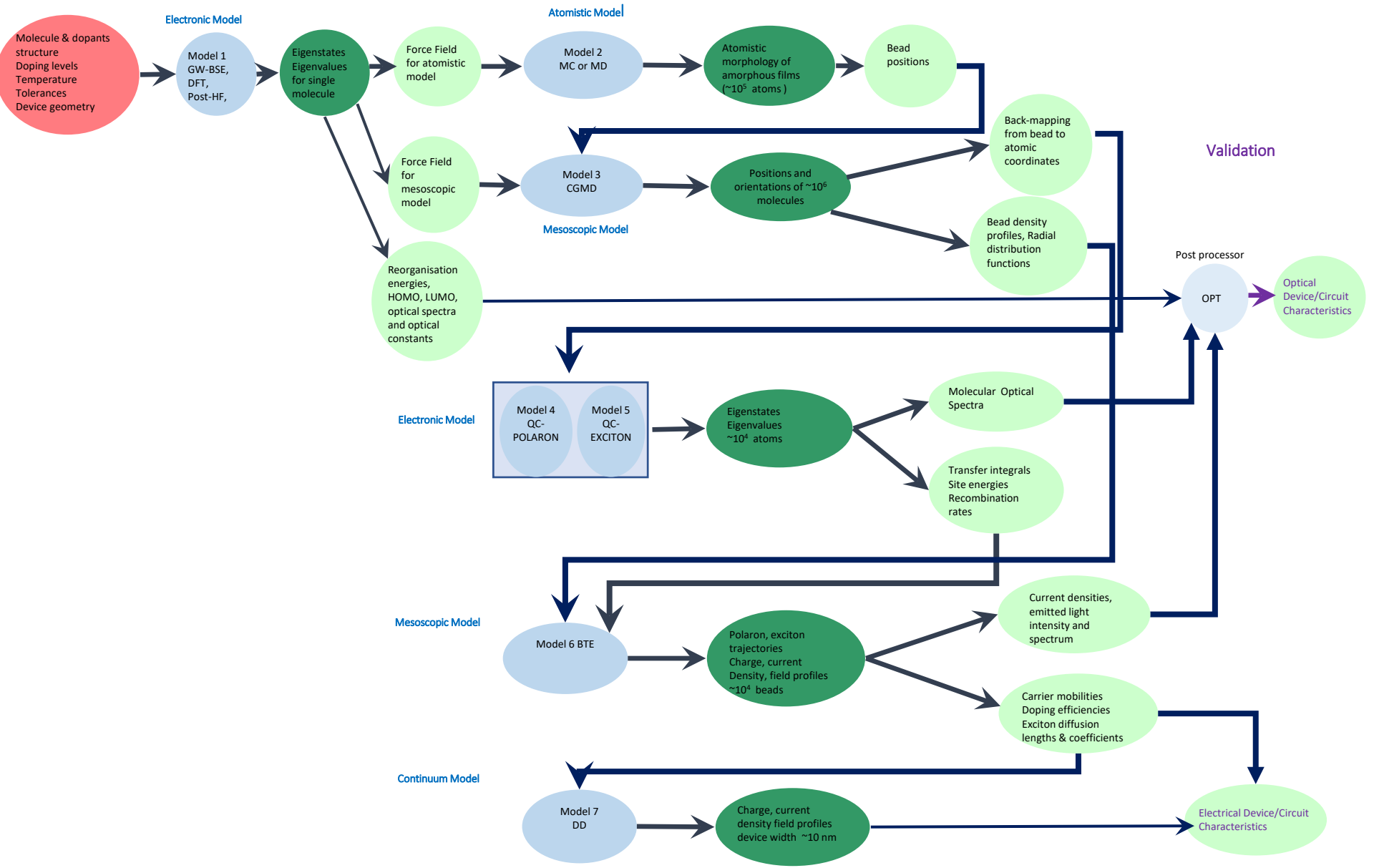
MAXWELL'S EQUATIONS (MHD approximation)

Flow fields, Species concentrations

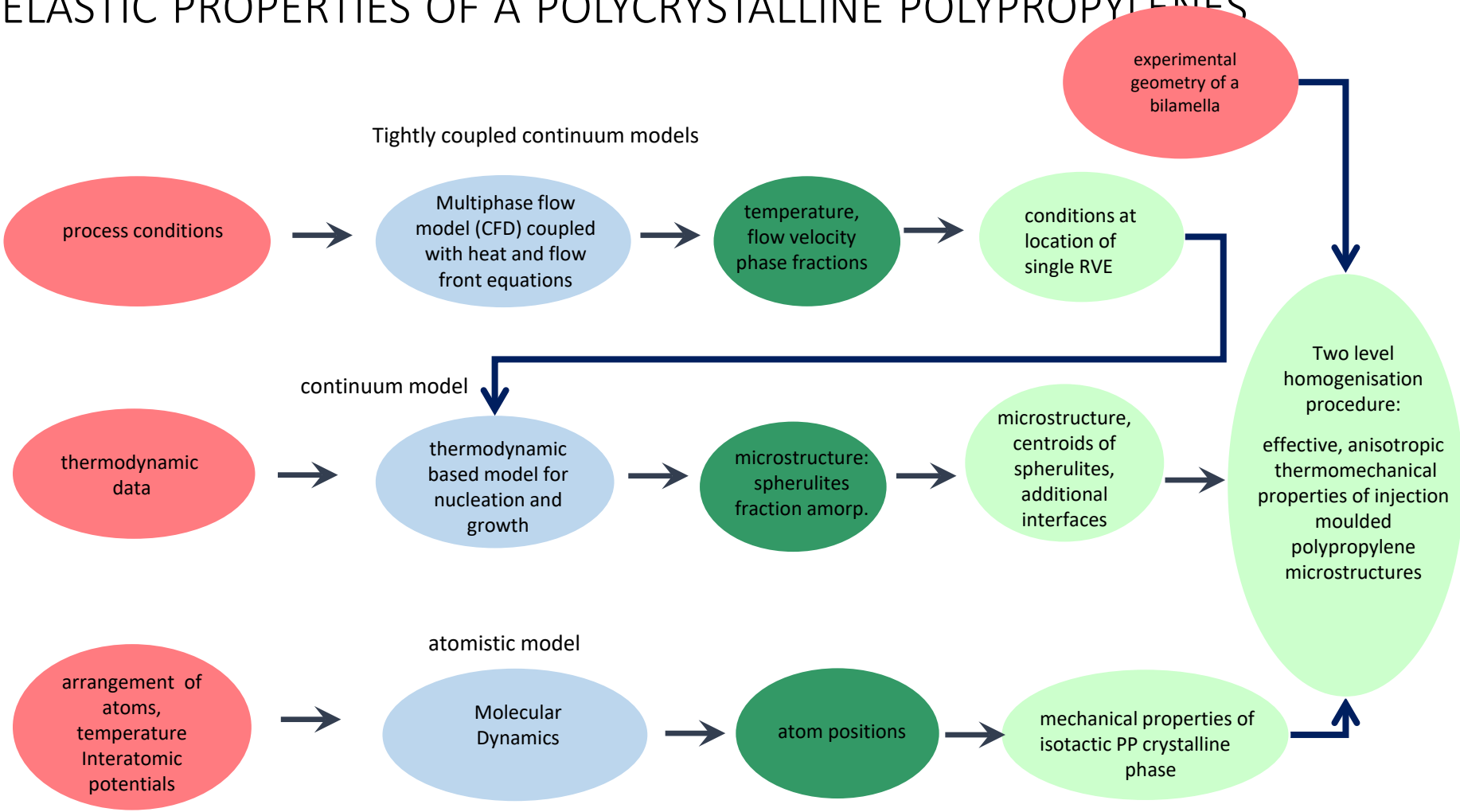
– Pressure
– Temperature
– Species concentrations

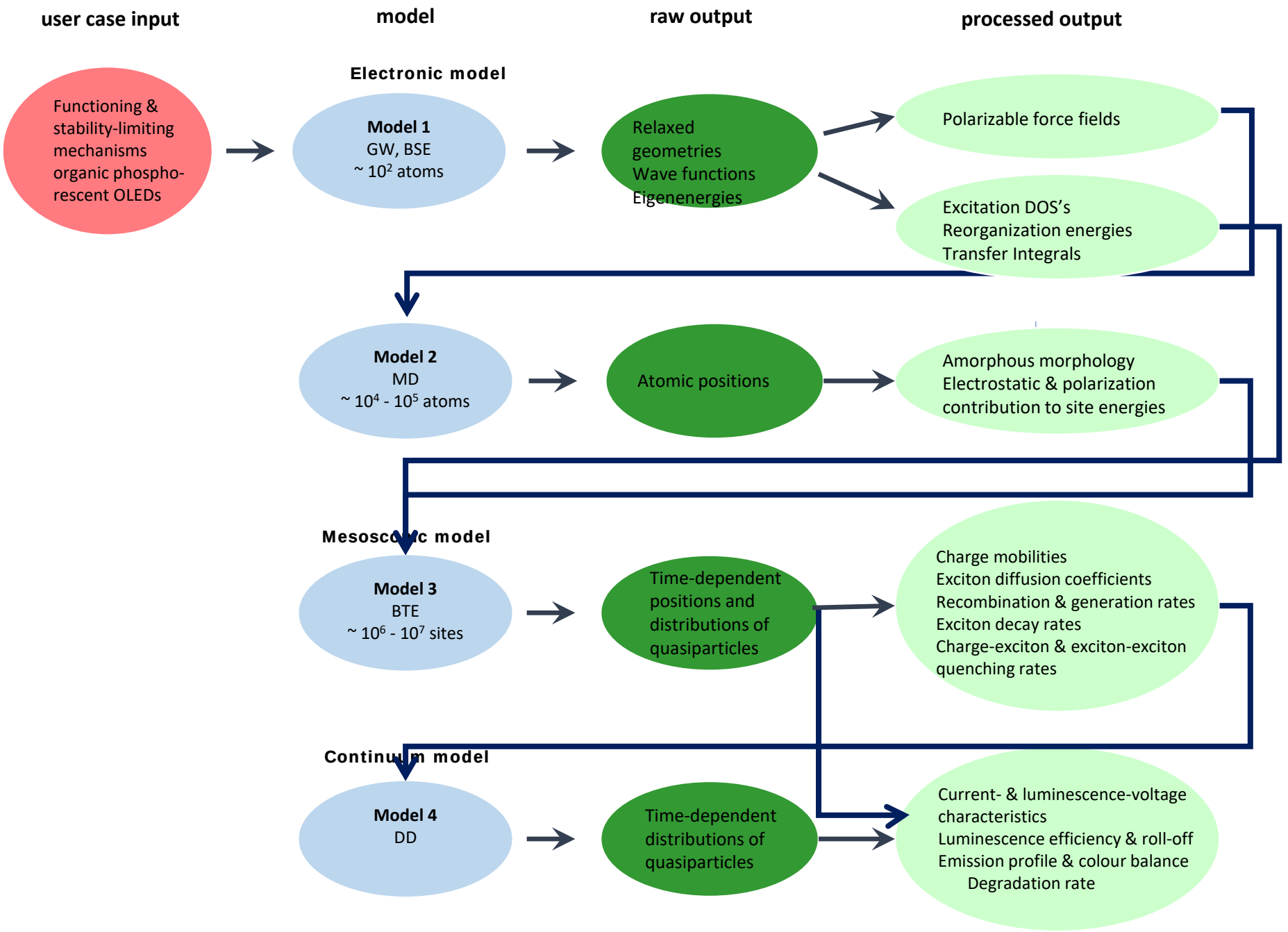
End User

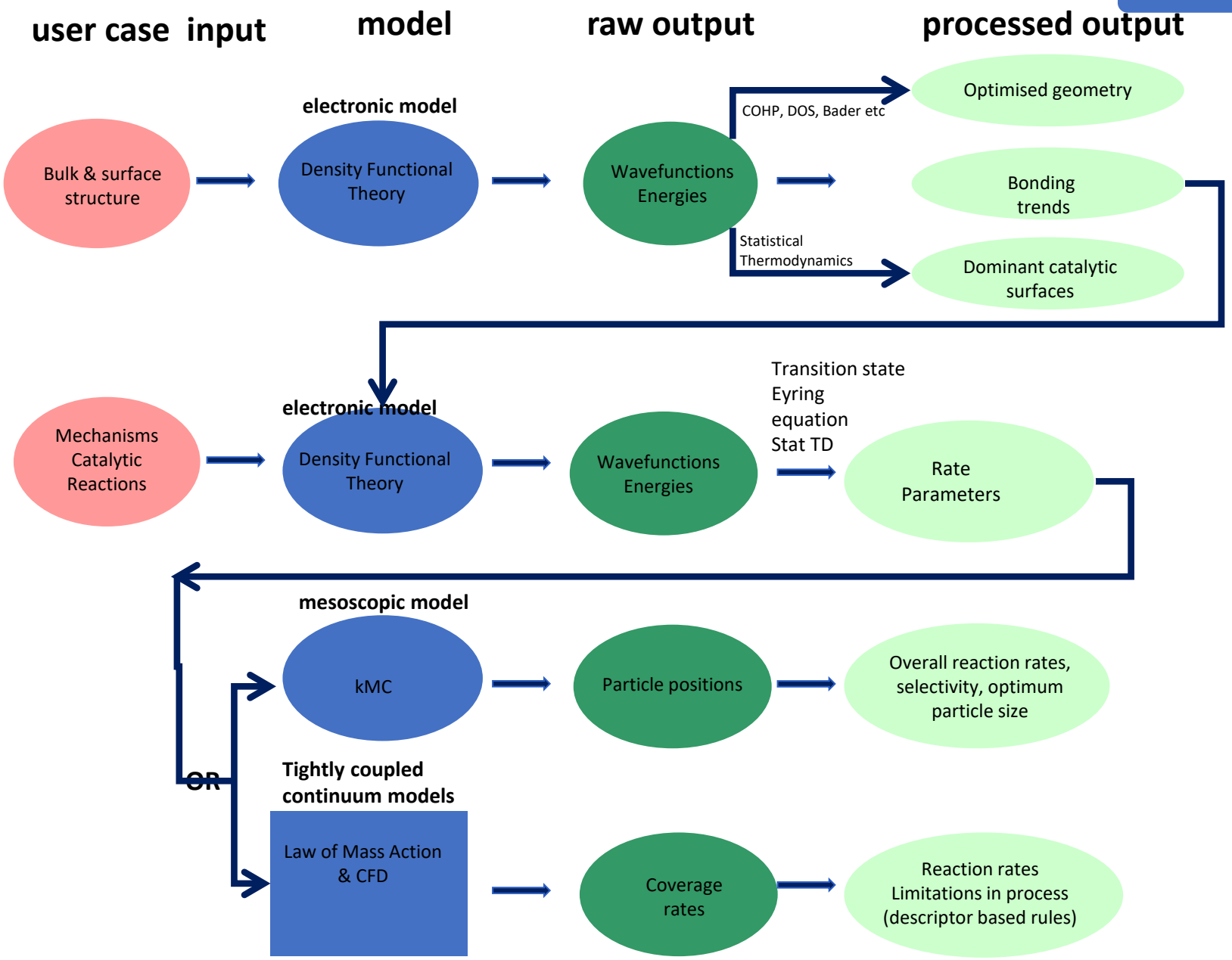
EXTMOS EXTended Model of Organic Semiconductors



ELASTIC PROPERTIES OF A POLYCRYSTALLINE POLYPROPYLENES




user case input
model
raw output
processed output
Functioning & stability-limiting mechanisms organic phospho-rescent 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


user case input
model
raw output
processed output
Bulk & surface structure
electronic model
Density Functional Theory
Wavefunctions Energies
COHP, DOS, Bader etc
Optimised geometry
Bonding trends
Statistical Thermodynamics
Dominant catalytic surfaces
Mechanisms Catalytic Reactions
electronic model
Density Functional Theory
Wavefunctions Energies
Transition state Eyring equation Stat TD
Rate Parameters
mesoscopic model
kMC
Particle positions
Overall reaction rates, selectivity, optimum particle size
OR
Tightly coupled continuum models
Law of Mass Action & CFD
Coverage rates
Reaction rates Limitations in process (descriptor based rules)

METADATA

RoMM taxonomy (vocabulary and classification) of material modelling
RoMM can be the basis for a top-level (upper) ontology (structure of knowledge)
MODA describes all aspects of a material simulation (workflow) with RoMM taxonomy

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)

EMMC PLANS FOR THE NEAR FUTURE

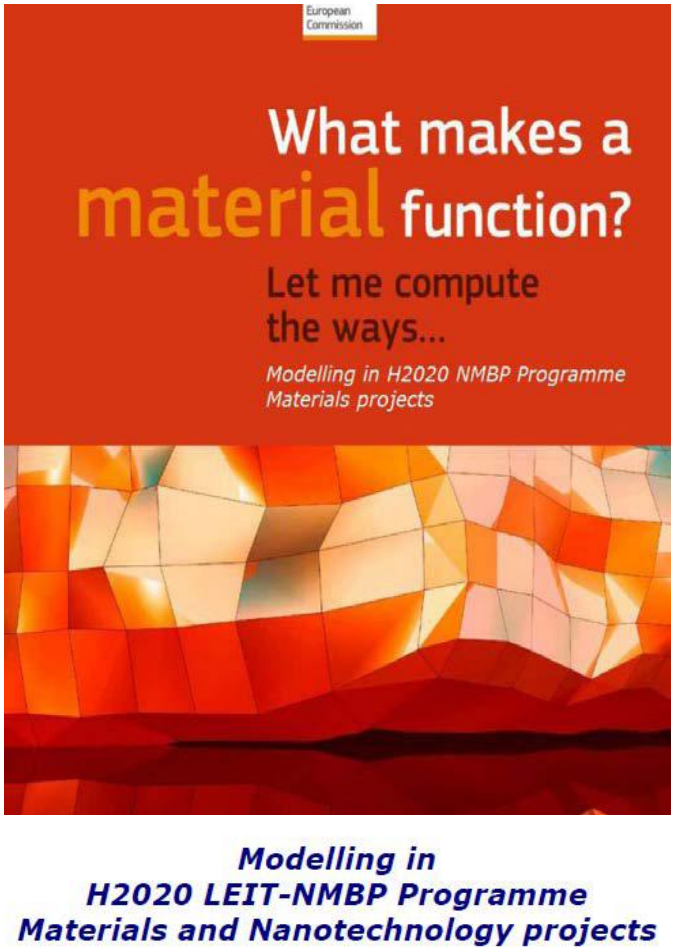
- Develop MODA online form for easy compilation, catalogue and formatting.
  - Distinguish between free text field entries (e.g. description) and fixed options (e.g. model entities)
  - Provide standard PE for the 24 model types so that every applicant will not need to reinvent the wheel
  - Provide 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

ACKNOWLEDGEMENTS

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)

https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0616197/

Short version of RoMM VI
https://bookshop.europa.eu/en/what-makes-a-material-function--pbKI0417104/