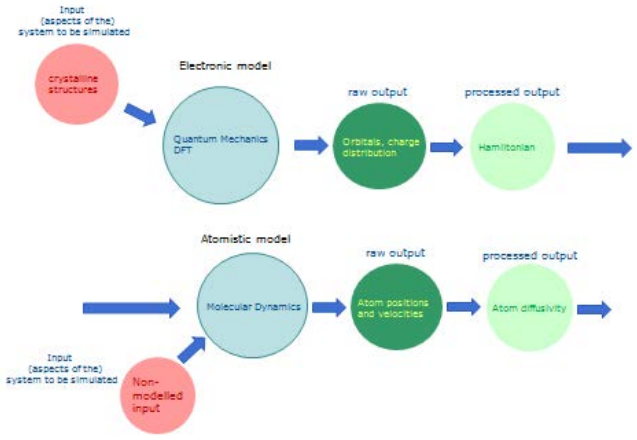
Elements in materials modelling

Each simulation will have its own MODA fiche.
Metadata for these elements are to be elaborated over time

Purpose of this document:
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the computational modelling details.

OVERVIEW of the simulation			
1	USER CASE	*General description of the User Case, please give the properties and behaviour of a particular material, material behaviour, manufacturing process or in-service-behaviour to be simulated. No information on the modelling should appear here.*	
2	CHAIN OF MODELS	MODEL 1	*Modelling projects consist of a chain of models, (workflow). All models should be identified as electronic, atomistic, mesoscopic or continuum and the related chapter in Review of Materials Modelling IV available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm) should be given.* *Please identify the first model*
		MODEL 2	*Please identify the second model*
		...	...
3	PUBLICATION ON THE SIMULATION	*Please give the publication which documents **the simulation** to indicate peer review and quality of the simulated data.*	
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 (including web link if available)*	



Workflow *(please replace the example)*

Textual rationale behind the choice of models and the workflow
The choice of which aspect of the user case is to be simulated with which model should be included

Each model used in a simulation can be documented in three chapters:

1. Aspect of the User Case or System simulated with this model
2. Model
3. Computation
4. Post processing

This processes the output of one simulation into input for the next simulation.

Please use the following four tables to document each "simulation with one model".
Coupled models can be written up collectively in one set of four tables.

Elements in the simulation with *< name the single materials model in the chain>*

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	*Describe the aspects of the user case textually.* *This is a like a description by an end-user who is not a modeller.* *Please keep all information on the models out of here.* *The next entries will appear in the pink circle of your workflow picture:*
1.2	MATERIAL	*Describe the chemical composition, …*
1.3	GEOMETRY	*Size, form, picture of the system (if applicable) (this is not the simulation box!)*
1.4	TIME LAPSE	*Femtoseconds, picoseconds, seconds, minutes, days…*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*If relevant, please list the process conditions (e.g. heated walls, external pressures and bending forces) to be simulated (if applicable).*
1.6	PUBLICATION ON THIS ONE SIMULATION	*Publication documenting **the simulation** with this single model (if available and if not 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 and only this will appear in the blue circle of your workflow picture.*	
2.1	MODEL ENTITY	*The entity in this materials model is <finite volumes, grains, atoms (phonons) or electrons>*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	*Name and description and mathematical form of the PE* *(or of the set of **tightly coupled** PEs)* *1. PE 1* *and in case set of **tightly coupled** PEs* *2. PE 2* *3. …*
		Physical quantities for each equation	*Please name the physics quantities (parameters (constants, matrices) and variables that appear in these equations e.g. wave function, Hamiltonian, spin, velocity, external force).* *1. Physics quantities of PE1* *and in case set of **tightly coupled** PEs* *1. Physics quantities of PE2* *2. …*
MATERIALS RELATIONS		**MR Equations**	*1. <Name of the material relation and which PE it completes>* *2. <Name of the material relation and which PE it completes >* *3. …*
		Physical quantities/ descriptors for each MR	*1. Name of the physics quantities, parameters (constants, matrices) and variables that appear in this MR1* *2. Name of the physics quantities, parameters (constants, matrices) and variables that appear in MR2* *3. …*
2.4	SIMULATED INPUT	*In case of sequential or iterative model workflows please document the simulated input and with which model it is calculated (note that what you enter will also appear in 4.1 of that respective model: this indicates that simulated output of the one model is input of the next)*	

This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	*e.g. Monte Carlo, SPH, FE, …*	
3.2	SOFTWARE TOOL	*(if own, please specify if can be shared, link to website/publication)*	
3.3	TIME STEP	*If applicable*	
3.4	COMPUTATIONAL REPRESENTATION *Refers to how your computational solver represents the material, properties, equation variables,*	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*Computational representation of the physics equation, materials relation and material (e.g. "written up for the entity in the model" or in the case of statistical approached "written up for finite volumes")*
		BOUNDARY CONDITIONS	*Describe the computational representation of the boundary conditions.*
		ADDITIONAL SOLVER PARAMETERS	*Pure internal numerical solver details that are often set* *1. Specific tolerances* *2. Cut-offs, convergence criteria* *3. Integrator options*

Post processing

The "raw output" calculated by the model is per definition the physics variable in the PE(s).
This is already specified in the entry 2.2 and will appear in your dark green circles in the workflow picture.
This output is processed by a post processor in order to calculate values for physics variables for larger entities that can be input to the next model or that are the final output of the total simulation.
The physics used to do this calculation is to be documented.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*The post processed output <…..e.g. calculated parameters, new MR > (will appear in your light green circles in the workflow picture and also in 2.4 of the next models MODA) calculated for the entity in the next model in the chain: electrons, atoms, grains, larger/smaller finite volumes…*
4.2	METHODOLOGIES	*Describe the physics used in this calculation (often volume averaging, thermodynamics)*
4.3	MARGIN OF ERROR	*Margin of error of property calculated <reasons and accuracy in percentages> that is of interest to an industry who wants to know the accuracy.*