The European Materials Modelling Council

MODA

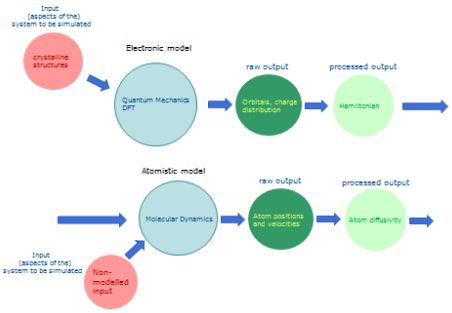
Modelling data documenting one simulation

Name <project, user-case, model>

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 the particular material, manufacturing process and/or in-service-behaviour to be simulated.*	
2	CHAIN OF MODELS	MODEL 1	*Please identify the first model*
		MODEL 2	*Please identify the second model*
		...	...
3	PUBLICATION ON THE SIMULATION	*Please give the publication which documents **this ONE simulation***	
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)*	
5	WORKFLOW AND ITS RATIONALE	*Please give a textual rationale of the choice of models and the workflow. This should include the choice of which aspect of the user case is to be simulated with which model.*	



Workflow

Each model used in this simulation can be documented in four chapters:

1. Aspect of the User Case or System simulated with this model
2. Model

Kommentar [DBA(1]: *Each simulation will have its own MODA fiche. Thus select one representative simulation and please do not try to demonstrate the wide applicability of your code.*

In case you do a series of independent simulations with the same model (like in high-throughput approaches to find the best material), you can list this set of user cases under 1.

Kommentar [DBA(2]: *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.*

Kommentar [DBA(3]: *Most 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.*

Kommentar [DBA(4]: *If there has been a peer review that this information can be indicated to underpin the quality of the simulated data.*

Kommentar [DBA(5]: *Please replace the example with your own*

Kommentar [DBA(6]: *Tightly c coupled models can be written up collectively in one set of four tables. Thisis only the case if one matrix is set up and solved in one go.*

Kommentar [DBA(7]: *Please make sure the notions Physics Equation and Materials Relation are properly understood. For continuum models the PE is often only the conservation equations coded up in bought software packages.*

3. Computational aspects
4. Post processing

< 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.*
1.2	MATERIAL	*Describe the chemical composition, …*
1.3	GEOMETRY	*Size, form, picture of the system (if applicable)*
1.4	TIME LAPSE	*Duration of the case to be simulated.*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*If relevant, please list the conditions 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 already included in the overall publication).*

Kommentar [DBA(8]: *This documents how the simulation specifications are translated into computer language.*

Kommentar [DBA(9]: *This documents how the output of one simulation is processed into input for the next simulation. This will show as the information given under 4.1 in the first model will be the same as the information under 2.4 "simulated input" for the next model. This is the essence of model inter-operability!*

Kommentar [DBA(10]: *Please name the single materials model in the chain you will now document in 4 chapters>*

Kommentar [DBA(11]: *The information in this chapter is end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture. This is disjunct from simulated input (see chapter 2.4) which would have been calculated by an other model.*

Sometimes pre-processing is necessary to translate the user case specifications to values for the physics variables of the entities. This relates to the pink circle of your workflow picture.

Kommentar [DBA(12]: *This is the description by an end-user who is not a modeller. Please keep all information on the models out of here.*

Kommentar [DBA(13]: *Please note that this is not the simulation box, which is to be documented in chapter 3.*

Kommentar [DBA(14]: *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.*

Kommentar [DBA(15]: *E.g. heated walls, external pressures and bending forces. Please note that these might appear as terms in the PE or as boundary conditions, but this will be documented in the relevant chapters.*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Model type and name **chosen from RoMM content list** (the PE).*	
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* *and ONLY in case set of **tightly coupled** PEs* *PE 2* *…*
		Physical quantities	*Please name the physics quantities in PE* *and ONLY in case set of **tightly coupled** PEs* *Physics quantities of PE2* *…*
2.3	MATERIALS RELATIONS	**Relation**	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 MR1* 2. *Name of the physics quantities, parameters (constants, matrices) and variables that appear in MR2* 3. *….*
2.4	SIMULATED INPUT	*please document the simulated input and with which model it is calculated.*	

Kommentar [DBA(16]: *This and only this will appear in the blue circle of your workflow picture. Please do not insert any other text but an indication of the MR is allowed.*

Kommentar [DBA(17]: *Other quasi-particles fall under this heading too.*

Kommentar [DBA(18]: *More than one PE can only appear if the tightly coupled equations are set up as one matrix which is solved in one go.*

Kommentar [DBA(19]: *Parameters (constants, matrices) and variables that appear in the equation e.g. wave function, Hamiltonian, spin, velocity, external force).*

Kommentar [DBA(20]: *This documents the interoperability of the models in case of sequential or iterative model workflows. It means that simulated output of the one model is input for the next . 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.*

This chapter 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	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	*Please give name and details*	
3.2	SOFTWARE TOOL	*Please give the name and if this is your own code, please specify if it can be shared, link to website/publication.*	
3.3	TIME STEP	*If applicable*	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, 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")*
		RELATIONS, MATERIAL	
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	*If applicable*	
3.6	ADDITIONAL SOLVER PARAMETERS	*Pure internal numerical solver details, If applicable, like* • *Specific tolerances* • *Cut-offs, convergence criteria*	

Kommentar [DBA(21]: *e.g. Monte Carlo, SPH, FE, …iterative, multi-grid, adaptive,…*

Kommentar [DBA(22]: 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)

Kommentar [DBA(23]: *Refers to how your computational solver represents the material, properties, equation variables,*

Kommentar [DBA(24]: Please note hat these can be translations of the physical boundary conditions set in the user case or they can be pure computational.

		• *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 circle in the workflow picture.

This output is often processed by a post processor in order to calculate values for physics variables for different entities that can be input to the next model. Or the output is homogenised for larger volumes in the form of a MR or Descriptor Rule that are the final output of the total simulation.
This will appear in your light green circle in the workflow picture and also in 2.4 of the next model.

The methodology (often including new physics) used to do this calculation is to be documented.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*Please specify the post processed output* *If applicable then specify the entity in the next model in the chain fro which this is calculated: electrons, atoms, grains, larger/smaller finite volumes.* *In case of homogenisation, please specify the averaging volumes.*
4.2	METHODOLOGIES	*Please describe the mathematics and/or physics used in this calculation.*
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.*

Kommentar [DBA(25]: *Output can be. calculated values for parameters, new MR and descriptor rules (that we in the RoMM do not call models!).*

Kommentar [DBA(26]: *In homogenisation this is volume averaging. But also new physics equations can be used to derive e.g. thermodynamics quantities or optical quantities from Quantum Mechanic raw output.*