Template for workflow modelling metadata

Modelling projects consist of chains of models. The chain can be introduced with:

1. The properties and behaviour of a particular material (textual description).
2. Description of the chain of models calculating these properties and behaviour (each model identified as electronic, atomistic, mesoscopic or continuum and by reference to a Chapter in Review of Materials Modelling IV available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm).
3. Publication documenting the workflow

Each model can be described by three chapters
1. Model detail
2. (part of the) industrial problem simulated
3. computational detail

Metadata for a single materials model

1. **Generic physics of the model equation (type of metadata: declarations)**
   <model type and name chosen from RoMM content list>
   1.1. This is a materials model for <entity: finite volumes, grains, atoms, electrons>
   1.2. The model has a physics/chemistry equation <name and description> that involve the following physics quantities < like wave function, Hamiltonian, spin, velocity, external force…>
   The model has a materials relation (closure/constitutive equation) <name of equatione> that involves the following physics quantities/descriptors <..>
   (Please just name the physics quantities (parameters (constants, matrices) and variables that appear in these equations). This is like a declaration of variables. This is for end-users to know what appears in the equations. And this "translates" to the implemented equation and its initial values)
   1.3 Publication documenting the model

2. **End-user problem/system that is simulated (type of metadata: declarations)**
   This is the "model application", "case to be studied".
   2.1. Specify material properties, behaviour and/or material manufacturing processes simulated. (Describe the case textually as if you were going to calculate it analytically. Think of exercises you did in the physics lessons: example: a person on a ladder on a slippery floor).
   2.2. Size, form, geometry, picture of the system and time lapse of the process
   2.3. Physics metadata for system that is simulated. Here should be listed
      - physics quantities that do not appear in the physics equation and not in the case description above but that are relevant to describe the system/problem/

Comment [AdB1]: •If you have a set of coupled equations then you need a separate fiche for this discrete model.

Comment [AdB2]: The idea is that the reason is given why certain concepts appear in the database.

Comment [AdB3]: E.g.MD thermostate: this is a physics condition and need thus be included in the PE.
It is funny, somebody else had the same question. It seems to me this is due to the fact that this condition can computationally be implemented in many different ways.
These different ways are to be described in Chapter 3. But the physics need to go in Chapter 1.

model application/case like e.g. density, external pressure, viscosity, chemical composition, impurities, mobility

- process conditions (like heated walls, external pressures, bending forces) to be simulated),

(Note this should not describe the output!)

2.4 Publication documenting the simulated case

3. **Computational modelling metadata for the case that is simulated (type of metadata: values/data)**

3.1 Numerical Solver: <description like Monet Carlo, SPH, FE>

3.2 Input you need to start computing, e.g. times step, number of "fictitious" particles (only in case this can be chosen freely like in Lagrangian solvers), grid size, computational boundary conditions, "fictitious" particle positions and velocities (that you can choose freely but are necessary to start computing).

3.3 Initialisation of all quantities and parameters (appearing in Ch1, Ch2, Ch3.1): (these are the code's input files and can for the moment remain empty until uploaded into a repository)

3.4 Keywords describing "raw output" calculated by the model for the entities

3.5 Keywords for "post processed properties" calculated for <entity: atoms, grains, finite volumes> from the raw output calculated with <please describe the post processor>

3.6 Margin of error of property calculated under 3.4

3.7 Publication documenting the simulation

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Comment [AdB4]: If you did not yet publish on this simulation then please leave it open.

Comment [AdB5]: Hhere we make a difference between an application with a specific number of particles, and computational numbers. In the first case they should be derived from the density given in 2.3 and they can not be ferely chosen.

Comment [AdB6]: Same comment

Comment [AdB7]: The idea is that different physics can be used to post-process and the chosen method should be presented . Averaging (when going to a coarser scale) is not always giving the right answer. E.g. when averaging temperature you might e.g. want to verify that the averaged temperature field is physical by applying the heat flow equation.
Somebody else might want to do postporocess differently. Going from coarse to fine even gives greater physics decisions to take! And these should be listed. Later on the raw data might turn out to be of quality, while the postpocessed data is not….

Comment [AdB8]: Think of an industry who wants to know what to expect in accuracy. Any description would be welcome