Materials Modelling in EC LEIT NMBP

The European Materials Modelling Council (EMMC)
Classification of models, workflow descriptions (RoMM V)
Requirements in WP 2016 and 2017 workflow and MODA

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STANDARDS AND REQUIREMENTS IN LEIT – NMBP ON PROPOSALS

TOWARDS A STANDARDIZED MATERIALS MODELLING VOCABULARY

Review of Materials Modelling (RoMM version V)

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

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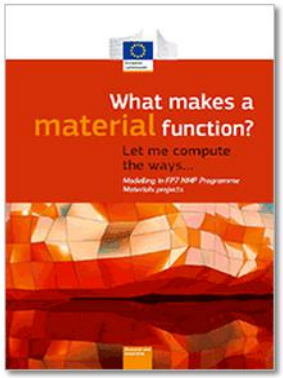
Review of Materials Modelling

(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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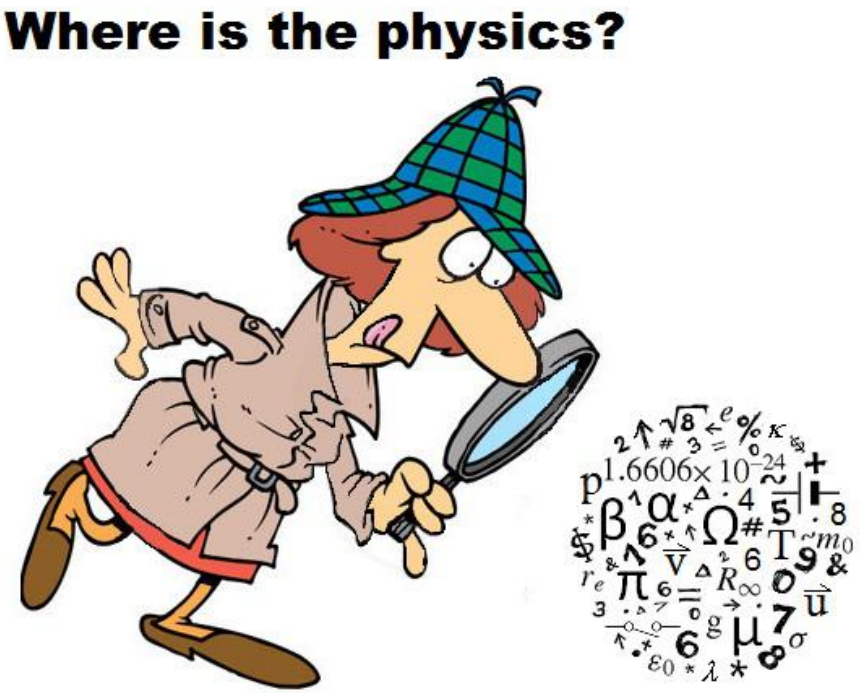
What non-informative descriptions do we find in proposals?

Often only the **phenomena (application)** is mentioned: "I have a mikro-kinetics model."
Or only the **scale** of the phenomena: "I have a mesoscale model."
Or only the name of the **software (code)** is mentioned: "I use the Uppsala model"
Or the model is named after the **solver**: "I have a FE model"

But…….

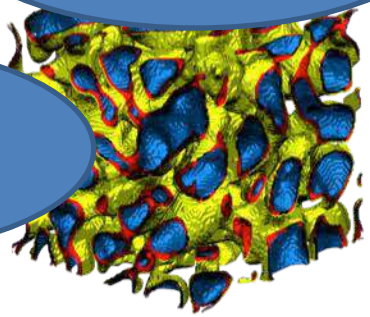


RoMM V

Fundamental entities and Forces Physics equations

Entities and Forces matter !!!

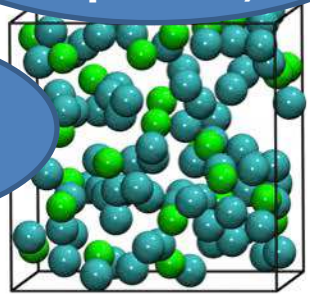
Conservation equations



Continuous Model

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

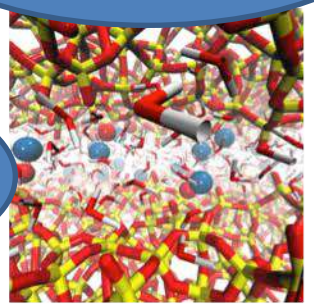
Diverse (e.g. Langevin equation)



Coarse Graining Methods

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

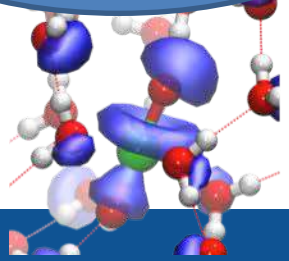
Newton equation



Molecular Dynamics Simulations

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

Schrödinger equation



Ab initio calculations

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

Entities matter ! Not size

A new way of building an overview of materials models.
Classification via the **entity** whose behaviour is described by the physics equation

1. electrons,
2. atoms,
3. nanoparticles/beads/grains
4. continuum finite volumes/elements

Models are strictly classified according to the entity whose behaviour is described by the physics equation in the model

not according to the size of the application or system
nor according to the lengthscale of the phenomena to be simulated

Entities and Forces! Not size

Materials Models (governing equations)

- physics or chemistry equations

  Generic equations describing the behaviour of electrons, atoms, particles or finite volumes (the model entities).

- materials relations

  Specifications of the specific material

A good way to find out the pertinent category of a model consists in discussing the

entities and their interacting forces

RoMM V

Solvers

Strict separation between solver and model

Solvers:

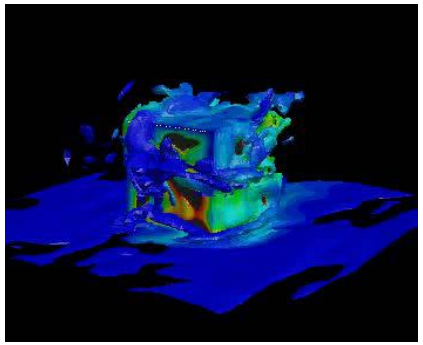
- SPH
- Kinetic Monte Carlo
- FEM
- DEM

"fictitious particles" and the entities whose behaviour is described.

Model class: Continuum
Physics Equations (list of models)

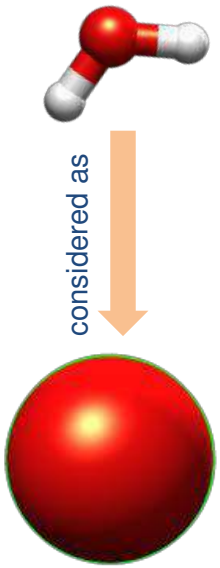
Consider the material to be homogeneous in finite volumes.
Write up a PE for the behaviour of these volumes:

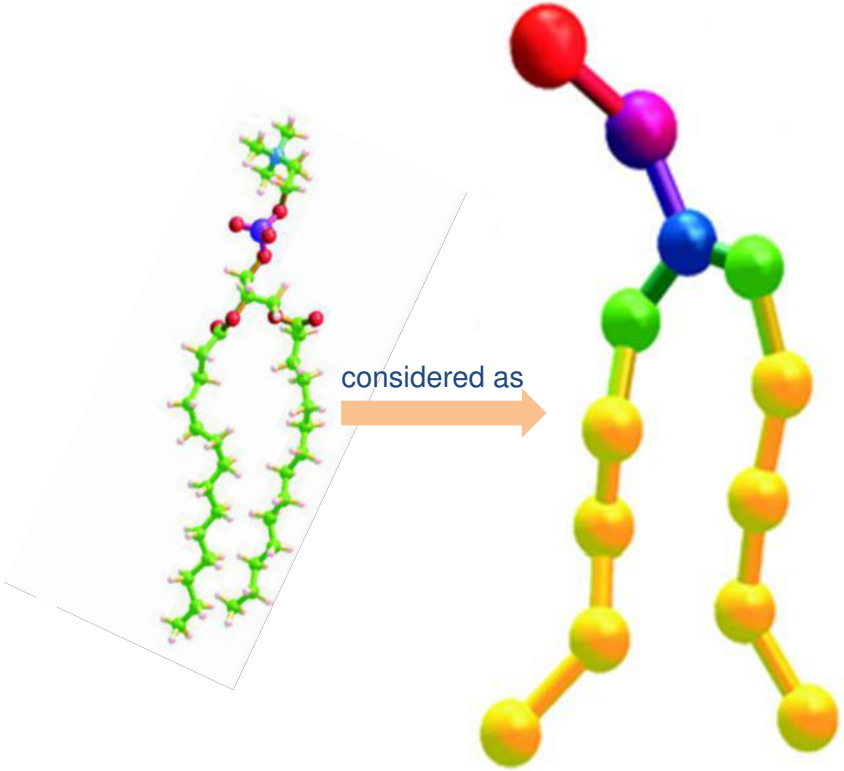
4.1 Solid Mechanics
4.2 Fluid Mechanics
4.3 Heat transfer and thermo-mechanics
4.4 Continuum thermodynamics and Phase Field models
4.5 Chemistry reaction (kinetic) models (continuum)
4.6 Electromagnetism (including optics, magnetics, electrical)
4.7 Process and device modelling



Model class: Mesoscopic models 1

Consider several atoms as one bead
Write up a Physics Equation for the behaviour/properties of this bead (or its distribution)





Model class: Mesoscopic models 2
Physics Equations

3.1 Mesoscopic (Dynamic) Density Functional Theory
3.2 Coarse Grained Molecular Dynamics
3.3 Discrete lattice dynamics model
3.4 Statistical Mechanics mesoscopic models
3.4.1 Dissipative Particle Dynamics (DPD)
3.5 Micro-magnetism model
3.6 Mesoscopic phonon models (Boltzmann Transport Equation)

Model class: Atomistic
Physics Equations (list of models)

Describe the behaviour of atoms:

2.1 Classical (Dynamic) Density Functional Theory
2.2 Molecular Mechanics
2.3 Statistical mechanics models: Molecular Dynamics
- 2.3.1 Classical molecular dynamics
- 2.3.2. Ab-initio molecular dynamics
- 2.3.3. Quantum mechanics/molecular mechanics (QM/MM)

2.4 Statistical mechanics models: Monte Carlo molecular models
2.5 Atomistic spin models
2.6 Statistical atomistic models
- 2.6.1 Langevin Dynamic method for magnetic spin systems
- 2.6.2 Semi-classical non-equilibrium spin transport model
- 2.6.3 Statistical transport model at atomistic level

2.7 Atomistic phonon models (Boltzmann Transport Equation)

Model class: Electronic Physics Equations (list of models)

Describe the behaviour of electrons:

1.1 Ab initio quantum mechanical (or first principle) models

- 1.1.1 Hartree Fock model
- 1.1.2 Higher level ab initio models
- 1.1.3 (Electronic) Quantum Density Functional Theory

1.2 Many-body models and effective Hamiltonians

- 1.2.1 Nearly free electron model
- 1.2.2 Pseudopotentials
- 1.2.3 Semi-empirical tight binding potential (TB) model
- 1.2.4 Hubbard model
- 1.2.5 k·p effective Hamiltonian
- 1.2.6 Polarisable continuum model
- 1.2.7 Envelope function approximation for continuous media

1.3 Quantum mechanical in response to time dependent fields

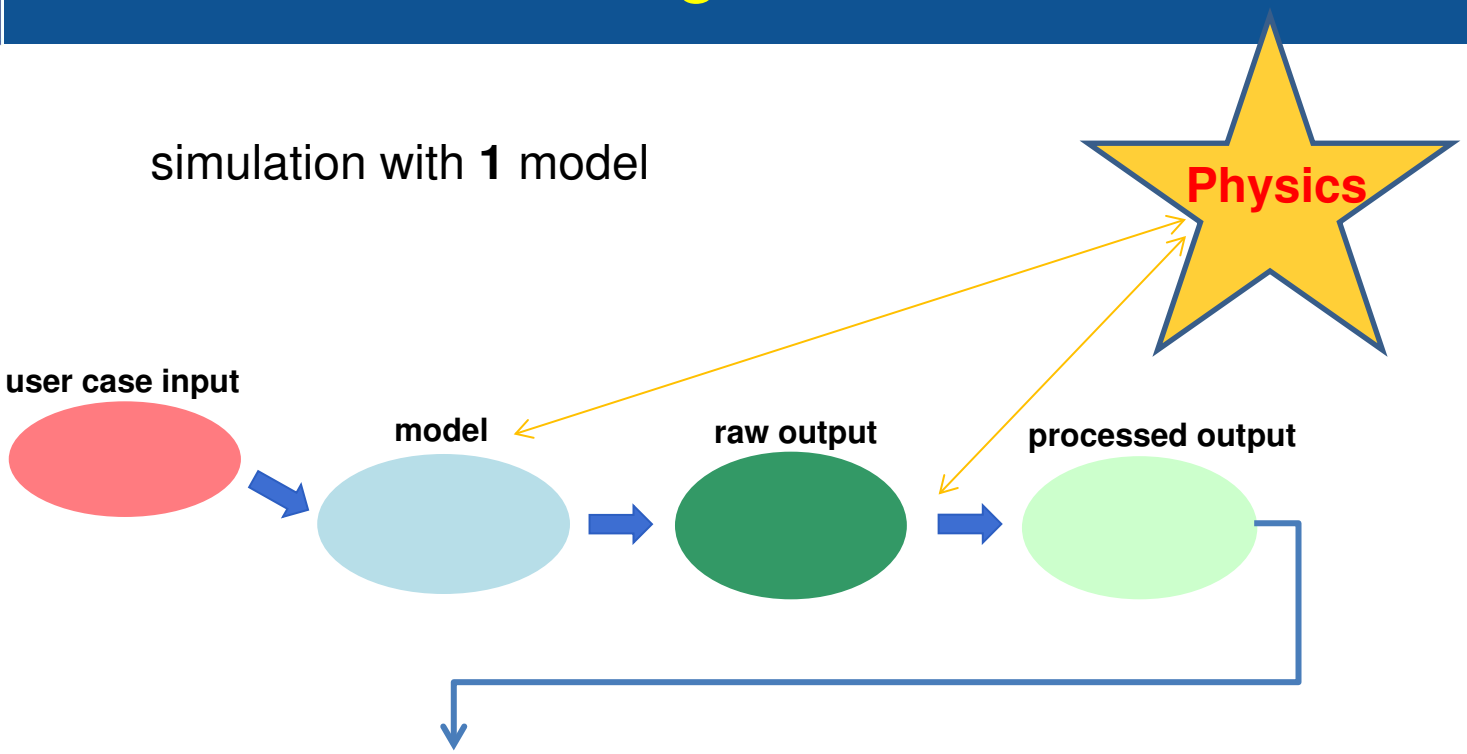
- 1.3.1 TD-DFT and TD(Spin)-DFT
- 1.3.2 Time dependent k·p model
- 1.3.3 Other time-dependent models

1.4 Statistical charge transport model

- 1.4.1 Semi-classical drift-diffusion model
- 1.4.5 Percolation models

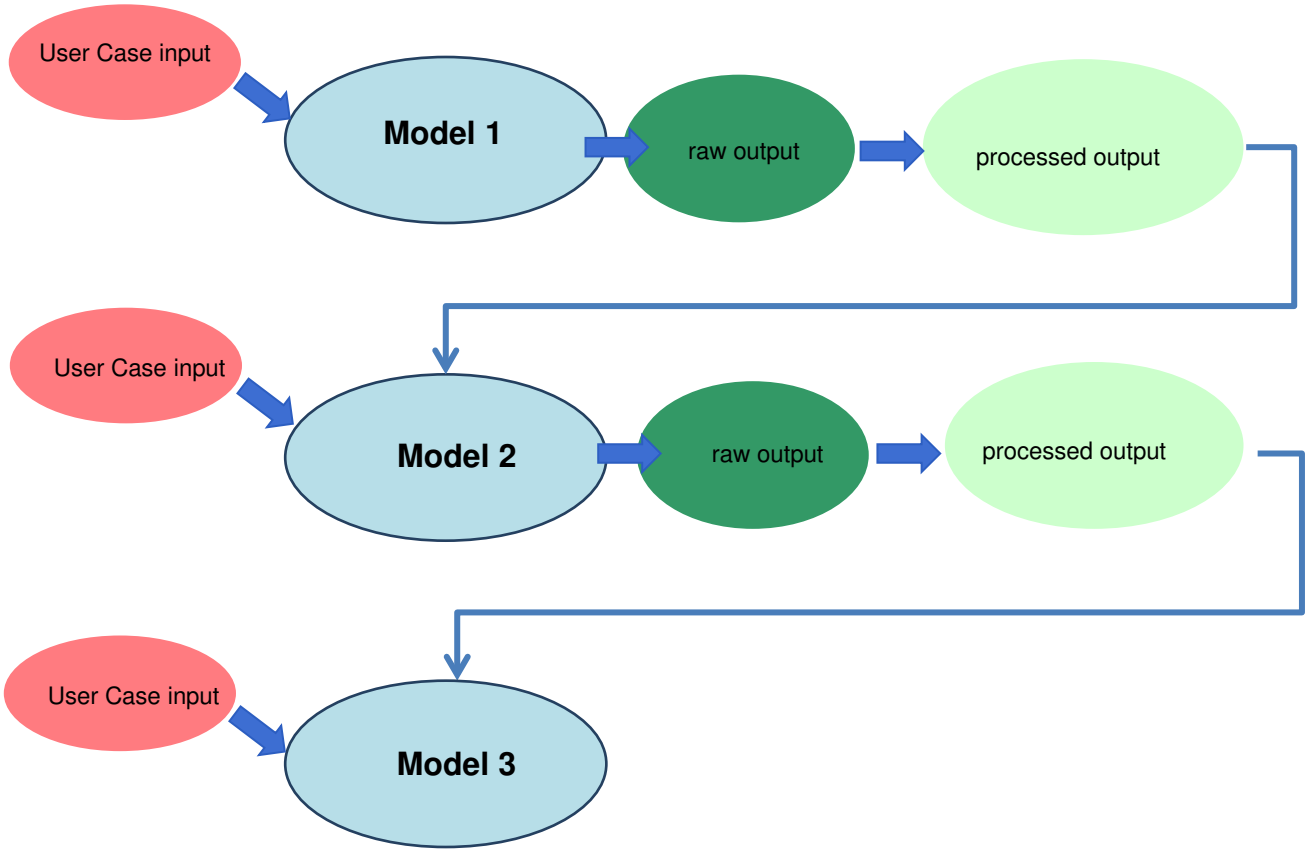
workflow building blocks

simulation with **1** model



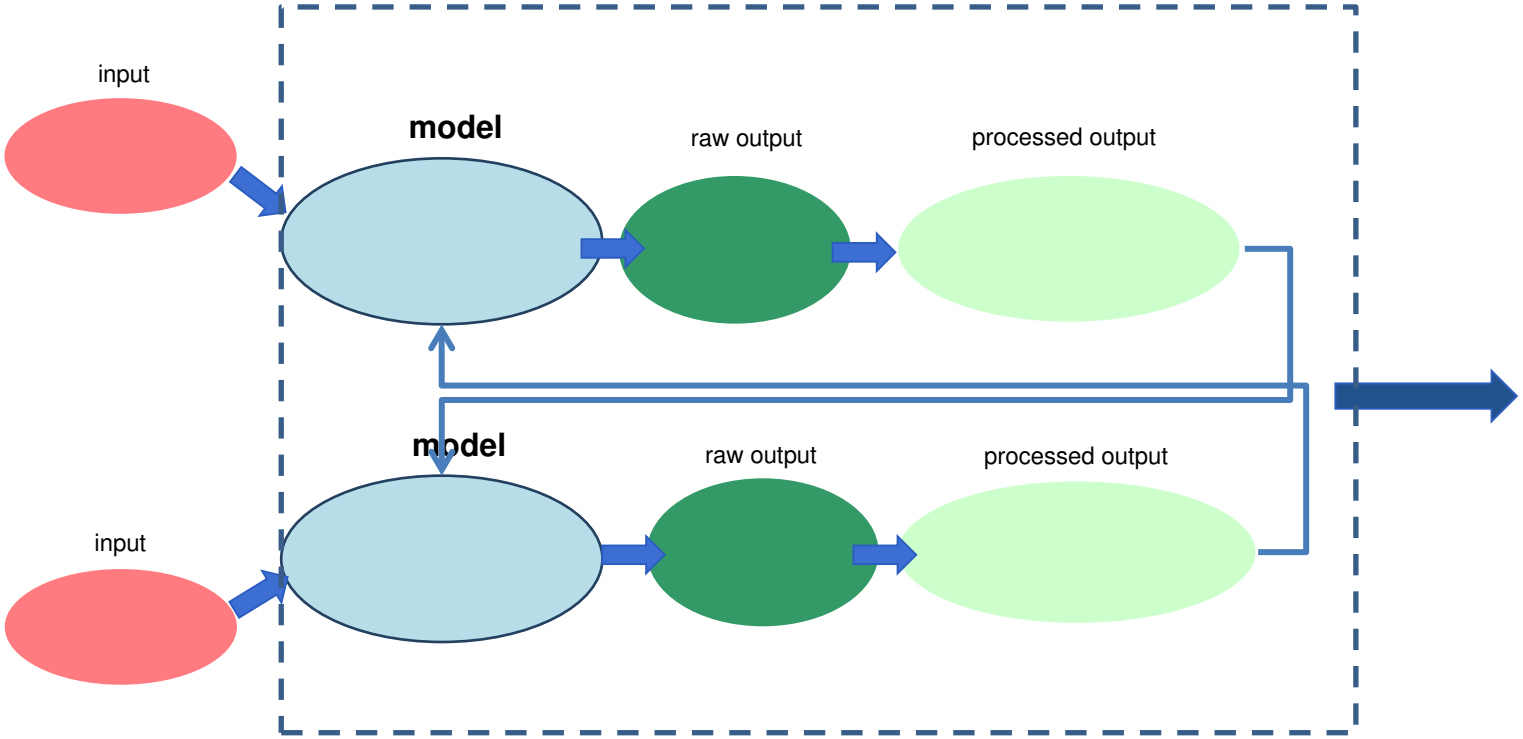
Interoperability: workflow template 1

Consecutive workflow: linked models

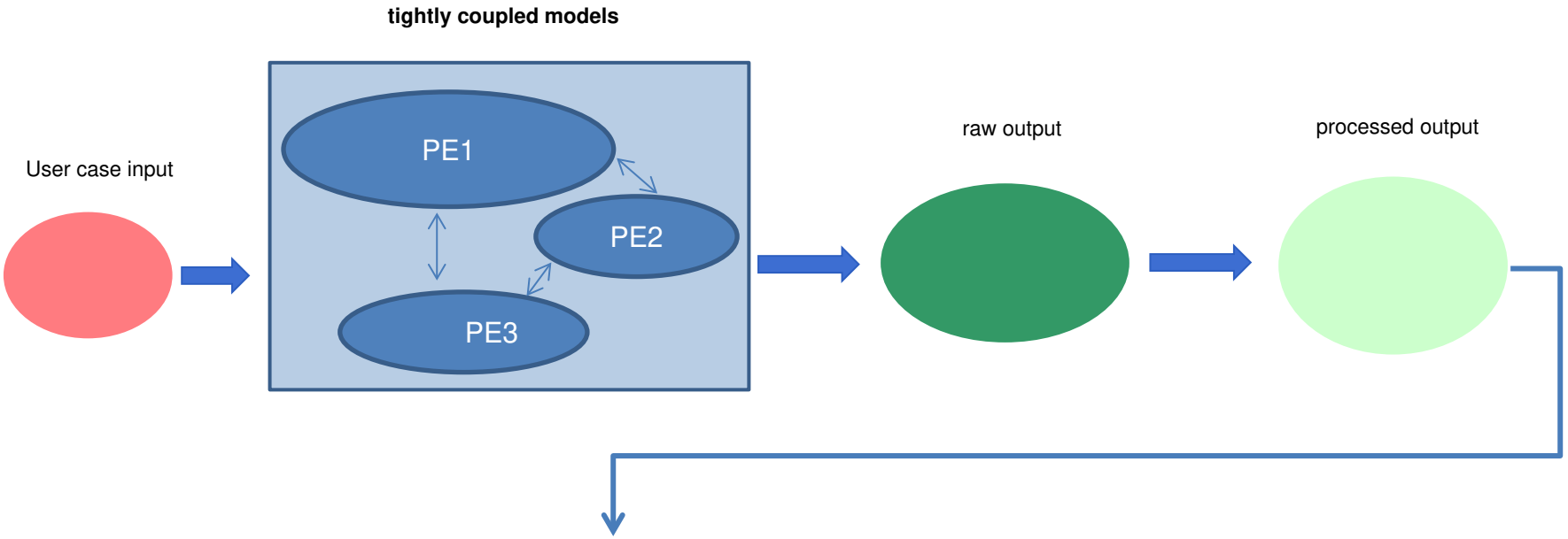


Interoperability: workflow template 2

Iterative workflow: iteratively linked models



Interoperability: workflow template 3

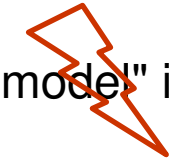


Tightly coupled models

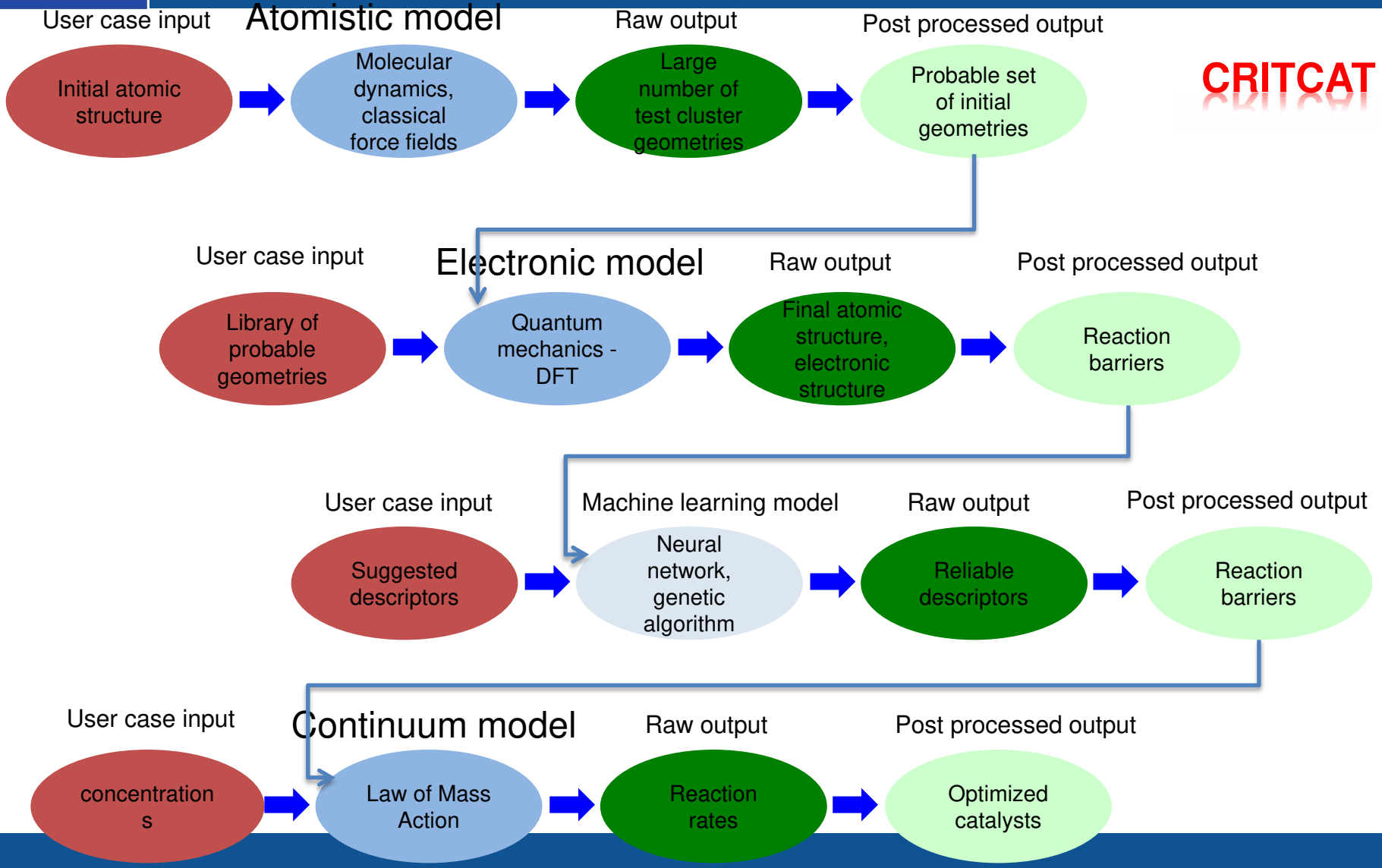
PEs that are represented by one matrix and solved in one go.

Three examples of different workflows for "microkinetics"
And there are thousands of combinations more possible!

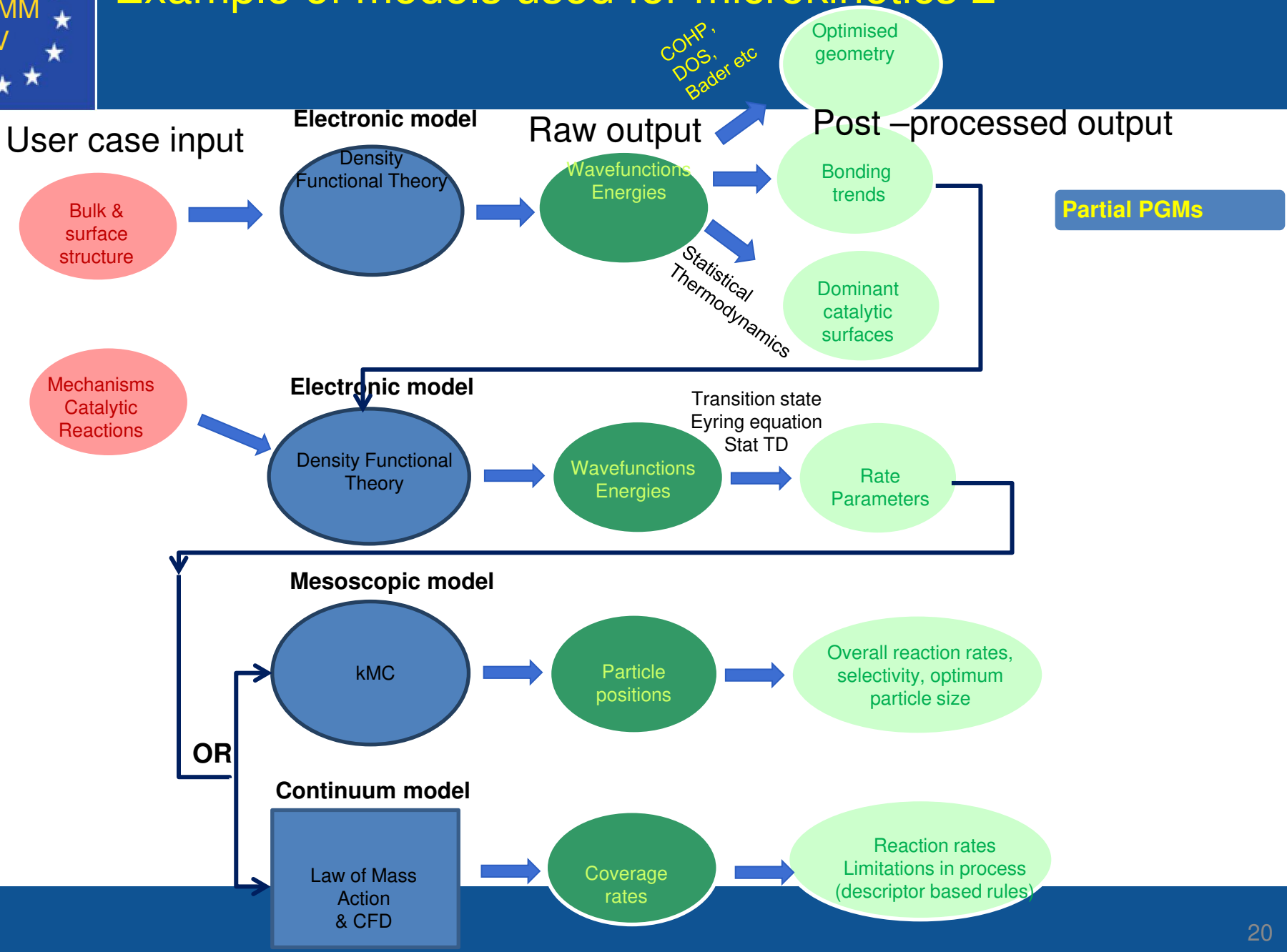
Thus the description "I have a microkinetics model" is non-informative!



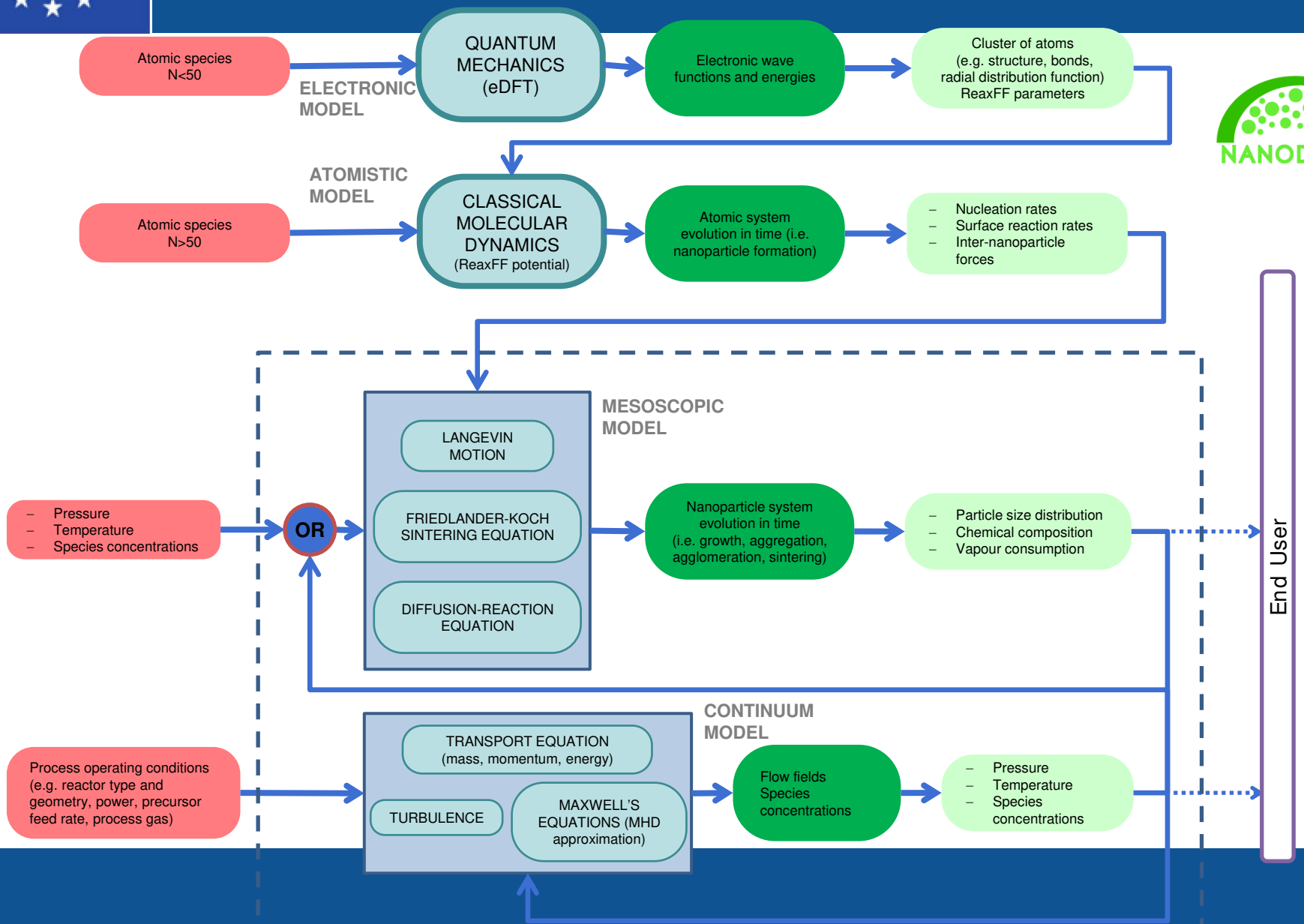
Example of models used for microkinetics 1



Example of models used for microkinetics 2



Example of models used for microkinetics 3



And if the use 14 models the number of possible combinations are endless

Classification of models
METADATA

These concepts (entities and forces (energy, potentials)) are proposed to be used as highest level metadata to describe models, databases

They are essential prerequisites for the ***interoperability*** of models (multi-scaling) and databases.

What does the NMBP programme expect in coming proposals?

INTRO TEXT LEIT-NMBP WP 2016-2017

WP 2016 and 2017 text:

1. *Where materials modelling is proposed, the relevant work packages should be described similarly to the Review of Material Modelling.*

2. *If new software is developed, software engineering quality measures should be addressed.*

3. *Proposers should consider participation in the open data pilot (mandatory for modelling topics NMBP 23, 24, 25) and*
4. *are encouraged to contribute actively to ongoing activities, e.g. in the EMMC (European Materials Modelling Council), and EU funded clusters.*

1. Descriptions of Modelling

Each proposal should present its **approach** to the modelling.
(approach is part of evaluation criterion 1).

The Review of Materials Modelling

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

should be followed to describe modelling.

This Review contains agreed vocabulary and template model workflows.

1. Descriptions of Modelling vocabulary

What are Models? What are Simulations? What are Codes? What are Solvers?

Materials Models consist of
"Physics Equations" **(PE)** and
"Materials Relations" **(MR)**
Together they are called governing equations.

Simulation is the execution of a model on an application (user case)
Software is a computational code, which solves the governing equations by numerical methods and requires information about the application (boundary and initial conditions)
Solvers are used to solve the physics/chemistry equation.

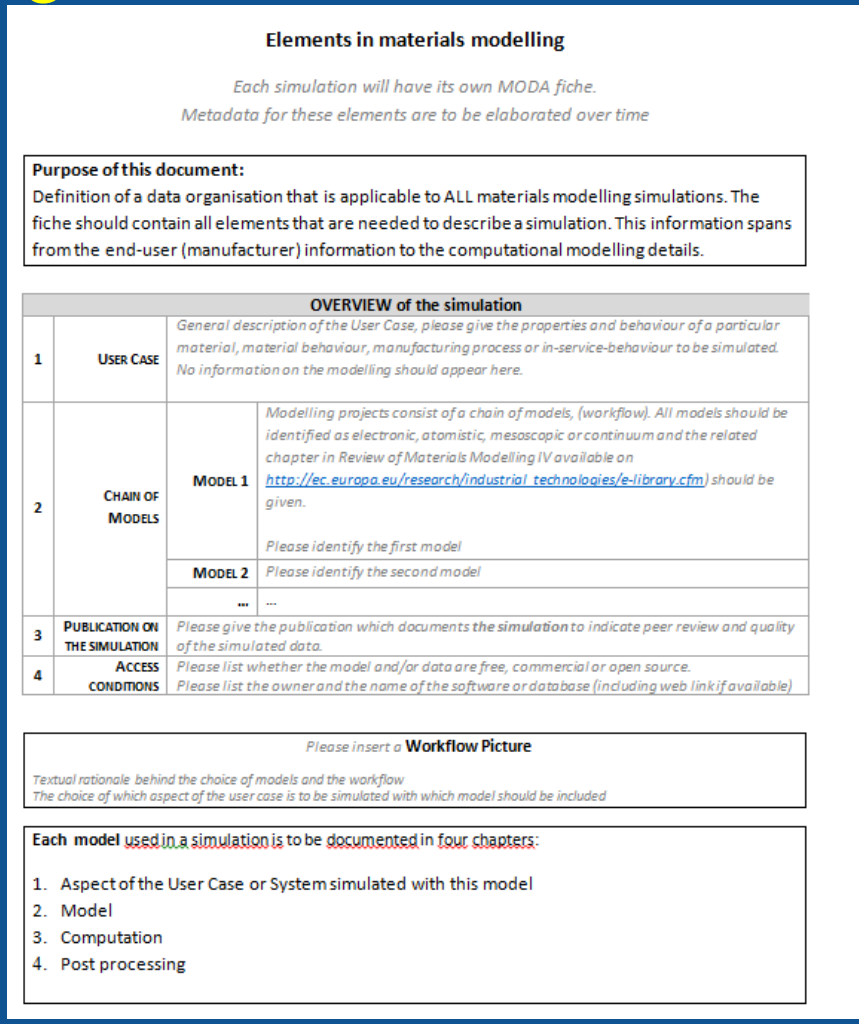
- **Models are not the codes; Codes contain much more than the model(s)**
- **Physics Equations have no length scales, thus models can not be named after length-scales**
- **Models should not be named after their solver; e.g. FE solver is used for 7 different PEs!**

1. Descriptions of Modelling

Workflow and MODA templates

Workflow and its components are explained in RoMM.
Examples of workflows on www.emmc.info

MODA are tables that take the modeller by the hand and ask the relevant questions step for step.



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)*	

Please insert a **Workflow Picture**

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 is to be documented in four chapters:

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

2. Software engineering guidance

Do not let a PhD student write disposable software!

Projects should develop re-usable software with a licence that allows industrial use.
A document elaborating this guidance can be found at www.emmc.info

3. Data management

All NMBP projects have to present data management
and this will be judged in evaluation criterion 3:
"effectiveness of the proposed measures
to manage research data where relevant "

Data management is necessary even when the Open Data Pilot is not obligatory!

All projects are encouraged to develop and apply metadata developed in the EMMC.

All projects are encouraged to participate in the **cataloguing of all simulations in Europe** in the Modelling Market Place of the EMMC (2017 Call).

4. Networking with EMMC

Many different tasks are undertaken in the EMMC:

Software owners
Manufacturers
Translators
Business decision support systems
Interoperability
Open simulation platform
Model development
Discrete models
Continuum models

Participation is encouraged

Dedicated, resourced **Networking** tasks are recommended to be included in the DoA.

Modelling
guiding and interpreting experiments

The interplay **modelling-characterisation** is always very strong.

The characterisation tools and properties to be measured are often well described, while the modelling tools and what aspect will be simulated are not (at all)
We request proper task descriptions!

Often proposals claim that "*modelling is guiding the experiments*".
For this to be realised, **deliverables should come early in the project!**

Often proposals claim "*modelling is used to interprete experimental results*".
For this to be realised, **deliverables have to be timed at characterisation time!**

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