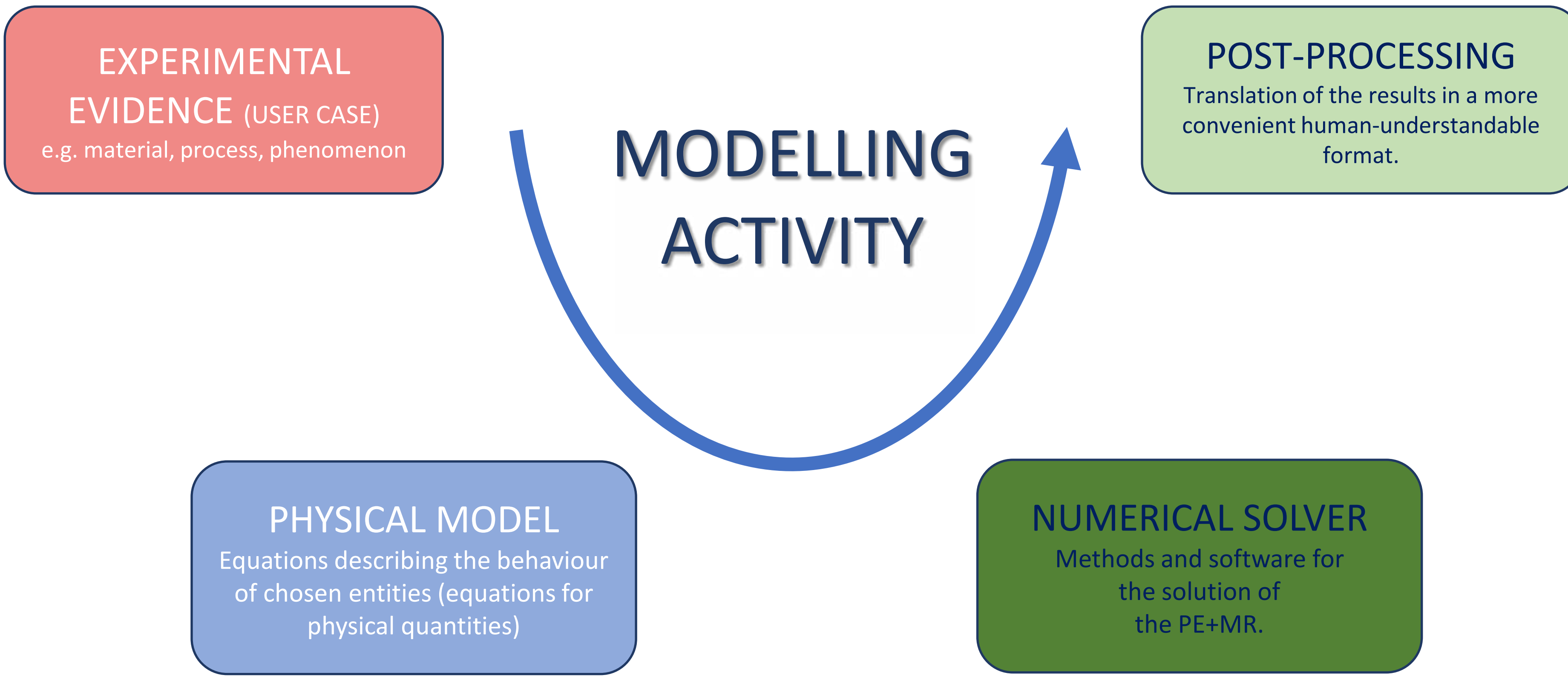
# MODA

## MODELLING DATA GENERALISATION:

# SUMMARY

- INTRODUCTION
- MODA TEMPLATE DESCRIPTION
- MODA CASE OF USE
- FUTURE STEPS AND FURTHER IDEAS




IT SEEMS A QUITE CLEAR, EASY AND STRAIGHTFORWARD PROCESS BUT …

# INTRODUCTION – COMPLEXITY

## … EACH BOX HIDES THE COMPLEXITY OF CASES, APPROACHES, METHODS.

(a user case can be treated in a multitude of different ways)

**EXPERIMENTAL EVIDENCE**

models can be applied to all situations which are experimentally measurable (i.e. everything)

**PHYSICS MODEL**

physics description for the same experimental evidence can differ depending on the choice of the model

**MATHEMATICAL REPRESENTATION**

mathematical representations of the same physics can differ, depending on the choice of physical quantities
e.g. energy or temperature for heat transfer

**NUMERICAL METHOD**

control volumes, finite elements, discrete elements, smooth particles, …

**NUMERICAL SOLVER**

several **methods** (e.g. iterative solvers) and **implementations** (e.g. BLAS, LAPACK)

**POST-PROCESSING**

*hic sunt leones…*

# INTRODUCTION – STAKEHOLDER INTERACTIONS

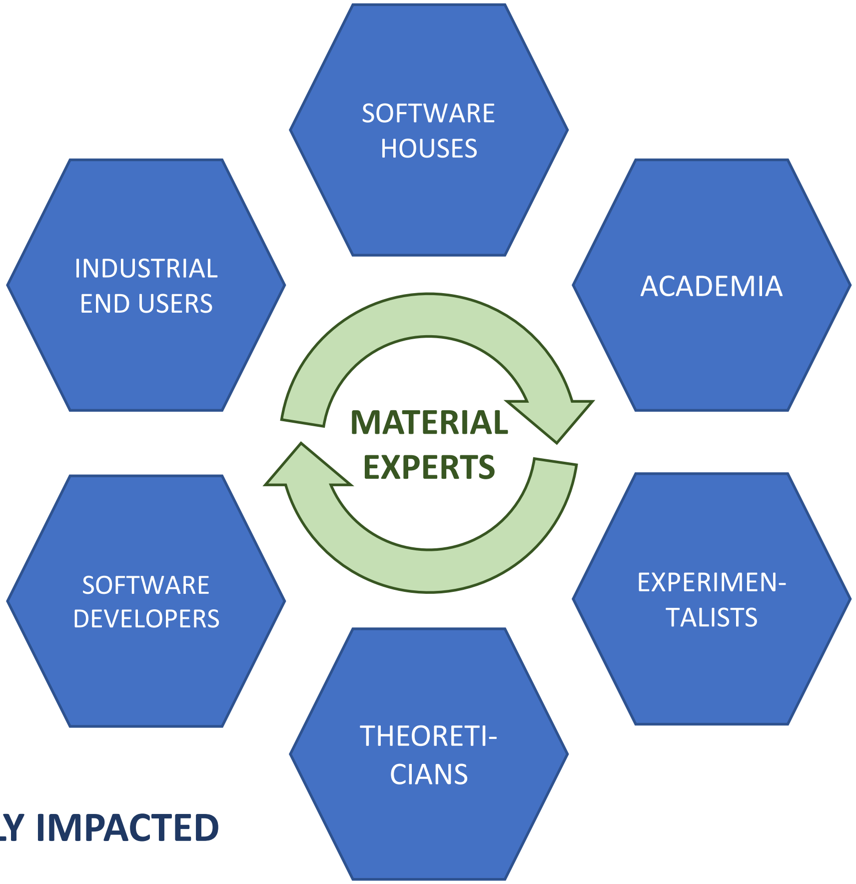
**INTERACTIONS** BETWEEN MATERIALS MODELLING **STAKEHOLDERS** IS OFTEN **THWARTED BY COMPLEXITY**.

OFTEN A MODELLING APPROACH IS ONLY **PARTIALLY DESCRIBED**, MENTIONING ONLY:

- PHENOMENA (e.g. microkinetics)
- SCALE (e.g. atomic, mesoscopic)
- SOFTWARE (e.g. LAMMPS, OpenFOAM)
- SOLVER (e.g. FEM, CV)

EACH COMMUNITY **HAS ITS OWN TERMINOLOGY**

**MULTI-SCALE** MATERIALS MODELLING THAT REQUIRES **MULTIDISCLIPLINARITY** AND **INTERACTIONS** BETWEEN DIFFERENT MODELS IS ESPECIALLY **ADVERSELY IMPACTED**

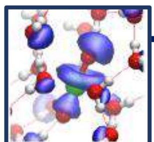



SOLUTION

ESTABLISH A **COMMON TERMINOLOGY** (DEFINITION OF **CONCEPTS** AND **VOCABULARY**) IN **MATERIALS MODELLING** WHICH WILL LEAD TO GREATLY **SIMPLIFIED** AND MUCH MORE **EFFICIENT COMMUNICATION**

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

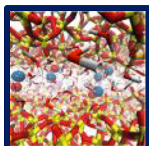
META-MODEL
( μετα → *beyond* )
the abstraction of the concepts in models (i.e. the model *class*)



AB INITIO

*Schrödinger equation*

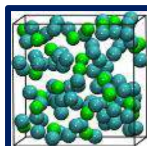
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$



MOLECULAR DYNAMICS

*Newton's law*

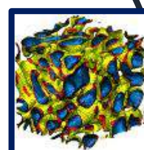
$$\frac{dV}{dr} = -m\frac{d^2r}{dt^2}$$



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

ATTRIBUTE

concept | vocabulary

In OOP this should be something like:

```
class Model {

      attribute_1;
      attribute_2;
      attribute_3;
      ...
}
```

Images from

# MODA - DEFINITION

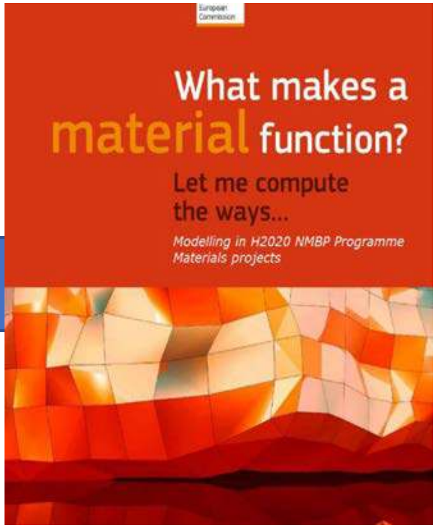
a first step in the direction of a standardised description of modelling has been taken by the EC

## 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** to the **computational details**.

It provides all necessary aspects for: **description, reproducibility, curation** and **interfacing** with other models.




***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 is based on the **core concepts** of

MODEL ENTITY

PHYSICS BASED MODELS

It includes also information about the **user case**, the **numerical solver** and **pre- and post processors**

IN THE **MODA**, MATERIALS MODELS ARE CLASSIFIED VIA THE

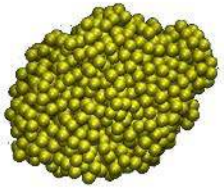
MODEL ENTITY → Self-contained, physically distinct, internally frozen, physical 'thing'

WHOSE BEHAVIOUR IS DESCRIBED BY PHYSICS

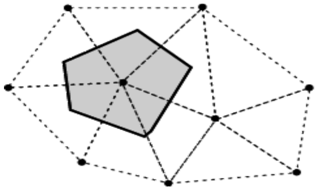
ELECTRONS

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.

**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 – Physical Based Models 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

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

### FLUID DYNAMICS

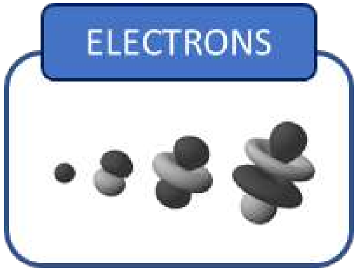
**PE** Navier Stokes equation

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

**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 – Model Types

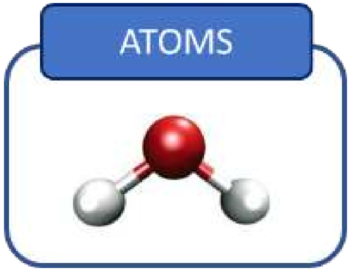



## Electronic Model

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of electrons 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*

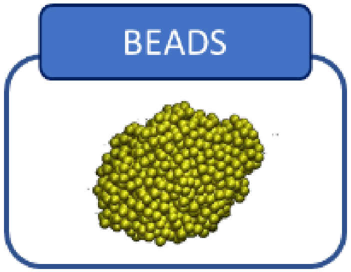



## Atomistic Models

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)*

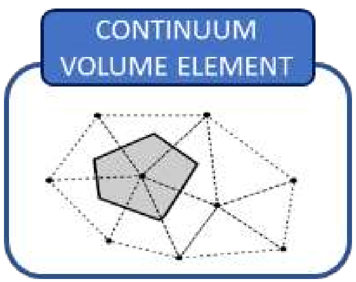
# MODA – Model Types




## Mesoscopic Models

Physics Based Model using a Physics Equation and Material Relation describing the behaviour of Beads either as 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)*
*4.7 Application of models to Processes and Devices*

# MODA – TEMPLATE STRUCTURE

## OVERVIEW OF THE SIMULATION

### MODEL 1

User Case | Model Physics

Solver | Post Processing

### MODEL 2

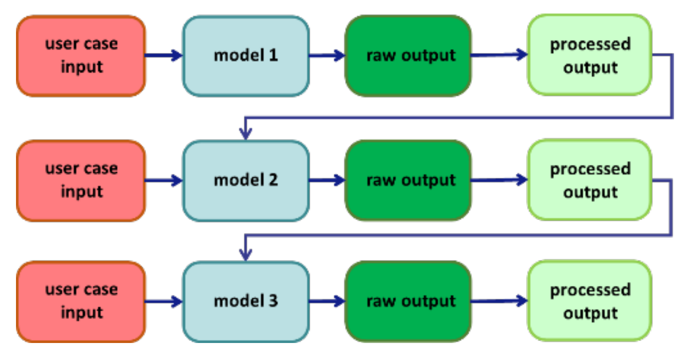
User Case | Model Physics

Solver | Post Processing

...

### MODEL n

### WORKFLOW



# MODA – TEMPLATE SNAPSHOTS

## HOW IT LOOKS!

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

| OVERVIEW of the SIMULATION | | | |
|---|---|---|---|
| 1 | USER CASE | | *General description of the User Case.*<br>*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.*<br>*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.*<br>*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.*<br>*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.*<br>*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)*<br>*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)*<br>*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.*<br>*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).*<br>*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).* |

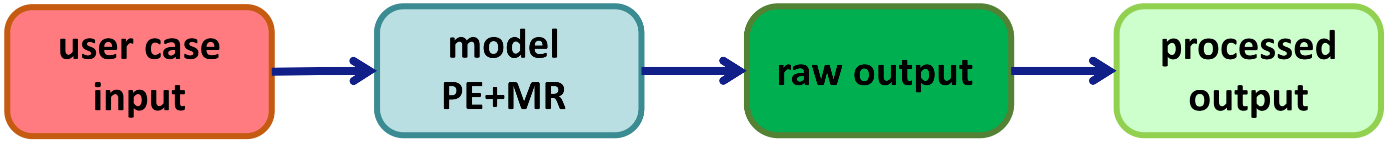
| 2 | GENERIC PHYSICS OF THE MODEL EQUATION | | |
|---|---|---|---|
| 2.0 | MODEL TYPE AND NAME | | *Model type and name* ***chosen from RoMM content list*** *(the PE).*<br>*This PE and only this will appear in the blue circle of your workflow picture. Please do not insert any other text although an 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*<br>*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.* |
| 2.3 | MATERIALS RELATIONS | **Relation** | *Please, give the name of the Material Relation and which PE it completes.* |
| | | **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.*<br>*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.*<br>*If you do simulations in isolation, then this box will remain empty.*<br>*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.*<br>*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.*<br>*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*<br>• *specific tolerances,*<br>• *cut-off, convergence criteria*<br>• *integrator options* |

| 4 | POST PROCESSING | |
|---|---|---|
| 4.1 | THE PROCESSED OUTPUT | *Please specify the output obtained by the post processing.*<br>*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.*<br>*In case of homogenisation, please specify the averaging volumes.*<br>*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.*<br>*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.* |

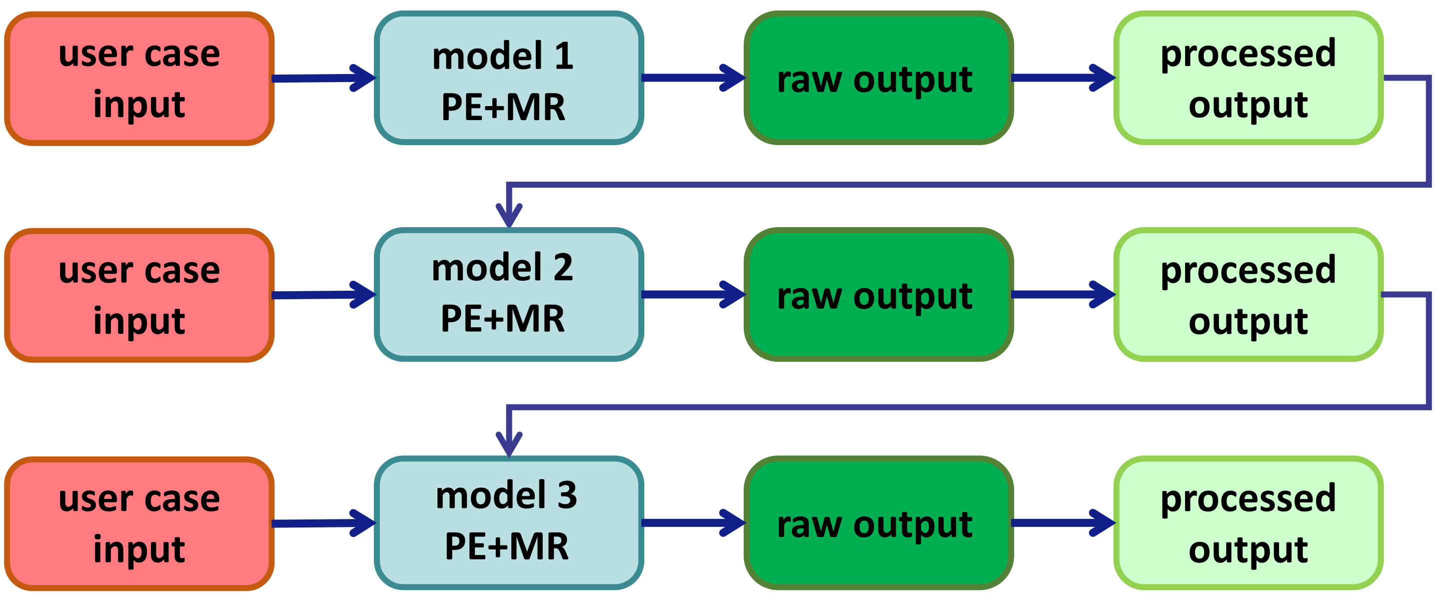
# MODA Workflow

## workflow for a **stand-alone model**



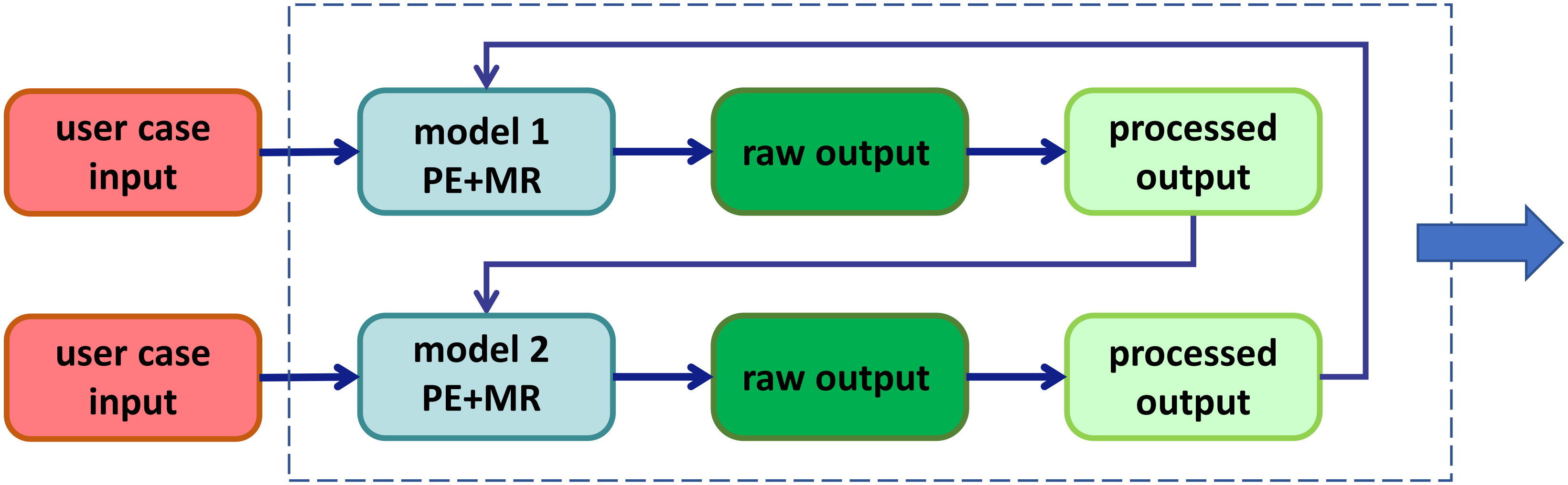

## workflow for a chain of **linked models**

equations solved sequentially
(i.e. one-way dependency)



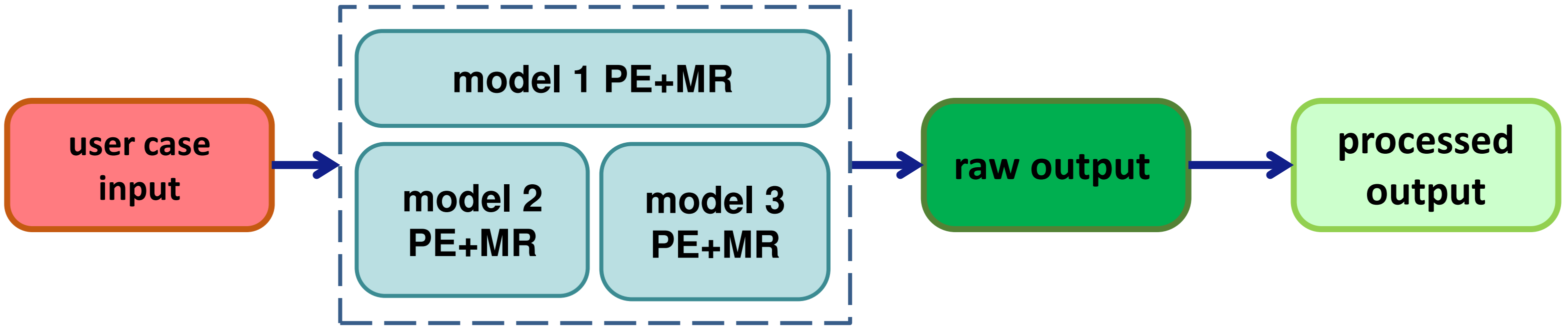
## workflow for a chain of **loosely coupled models**

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

<table>
<tr><th colspan="3">OVERVIEW of the SIMULATION</th></tr>
<tr><td>User Case</td><td colspan="2">General description of the User Case: properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated.<br>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.</td></tr>
<tr><td rowspan="5">Chain of Models</td><td>Model 1</td><td rowspan="4">Please identify all models used in this simulation. Note these are assumed to be physics-based models unless it is specified differently.<br>Most modelling projects consist of a chain of models (workflow).<br>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.</td></tr>
<tr><td>Model 2</td></tr>
<tr><td>…</td></tr>
<tr><td>Model N</td></tr>
<tr><td>Data-Based Model</td><td>If data-based models are used, please specify.</td></tr>
<tr><td>Publication Peer-Reviewing the Data</td><td colspan="2">The publication which documents the data of this ONE simulation.<br>This article should ensure the quality of this data set (and not only the quality of the models).</td></tr>
<tr><td>Access Conditions</td><td colspan="2">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).</td></tr>
<tr><td>Workflow and its Rationale</td><td colspan="2">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.<br>This should include the reason why a particular aspect of the user case is to be simulated with a particular model.</td></tr>
</table>

# 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/System to be Simulated** | |
| | **Aspect of the User Case to be Simulated** | *Describe the aspects of the User Case **textually**.*<br>***No modelling information** should appear in this box. This case could also be simulated by other models in a benchmarking operation!*<br>*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.*<br>***Simulated input** which is calculated by another model **should not be included**.*<br>*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.*<br>*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).*<br>*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 Equation | | |
|---|---|---|
| **Model Type and Name** | | *Model type and name* ***chosen from RoMM content list****.* <br> *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*** <br> *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.* <br> *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.* <br> *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.*<br>*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.*<br>*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.*<br>*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).*<br>*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.*<br>*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 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**
**Data-based Model**

**MODEL X**

| | | |
|---|---|---|
| **1** | **User case:** | |
| 1.1 | Aspect of the User Case to be calculated | |
| 1.2 | Material | |
| 1.3 | Geometry | |
| 1.4 | Time Lapse | |
| 1.5 | Manufacturing process or in-service conditions | |
| 1.6 | Publication on this one datamining operation | |

| | | | |
|---|---|---|---|
| **2** | **The Data-based Model** | | |
| 2.0 | Equation type and name | *e.g. energy minimizer* | |
| 2.1 | Database and type | *e.g. thermodynamic database CALPHAD*<br>*e.g. simulated data with DFT model and experimental data from AFM* | |
| 2.2 | Equation | Hypothesis | *The hypothetical relation assumed* |
| | | Physical quantities | |

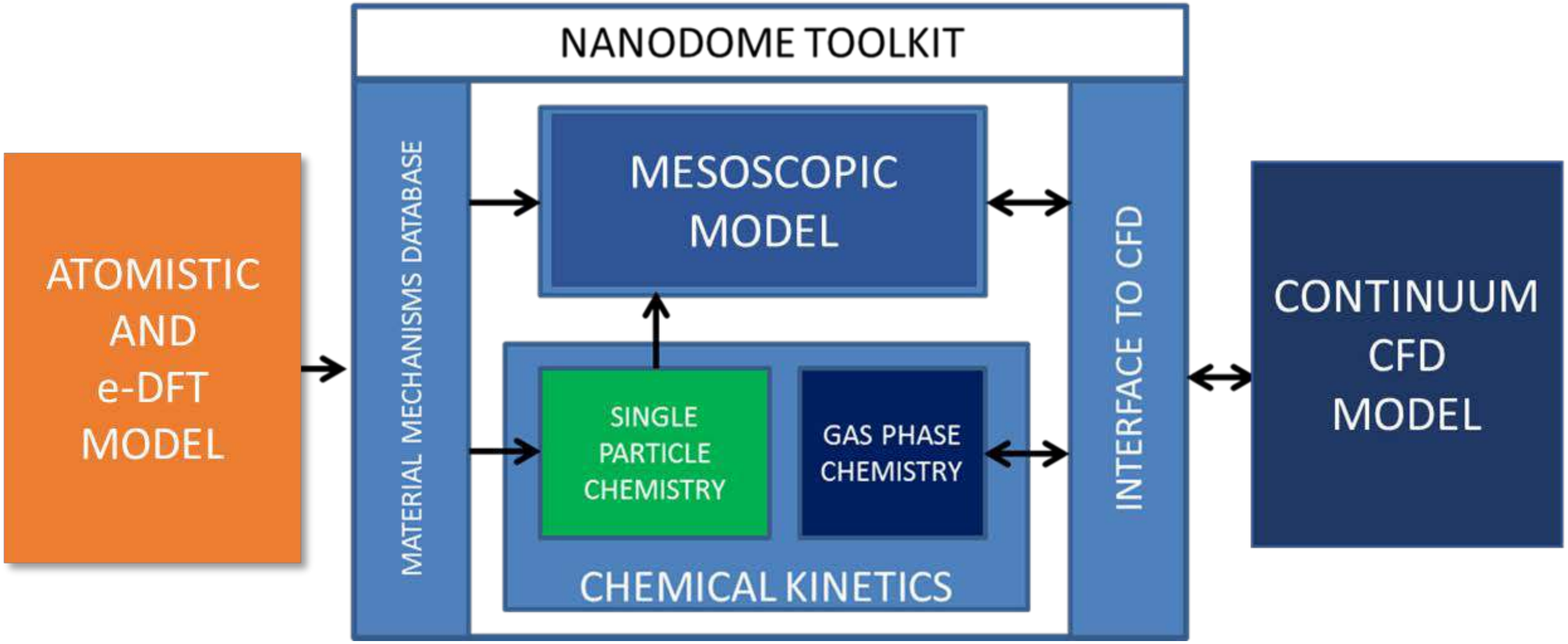
| | | |
|---|---|---|
| **3** | **Computational detail of datamining operation** | |
| 3.1 | Numerical Operations | |
| 3.2 | Software tool | |
| 3.3 | Margin of Error | |

# NANODOME

## Nanomaterials via **Gas-Phase Synthesis**:
## A Design-Oriented Modelling and Engineering Approach

*NanoDome* project has received funding form the European Union's *Horizon 2020 Research and Innovation Programme*, under Grant Agreement n° 646121

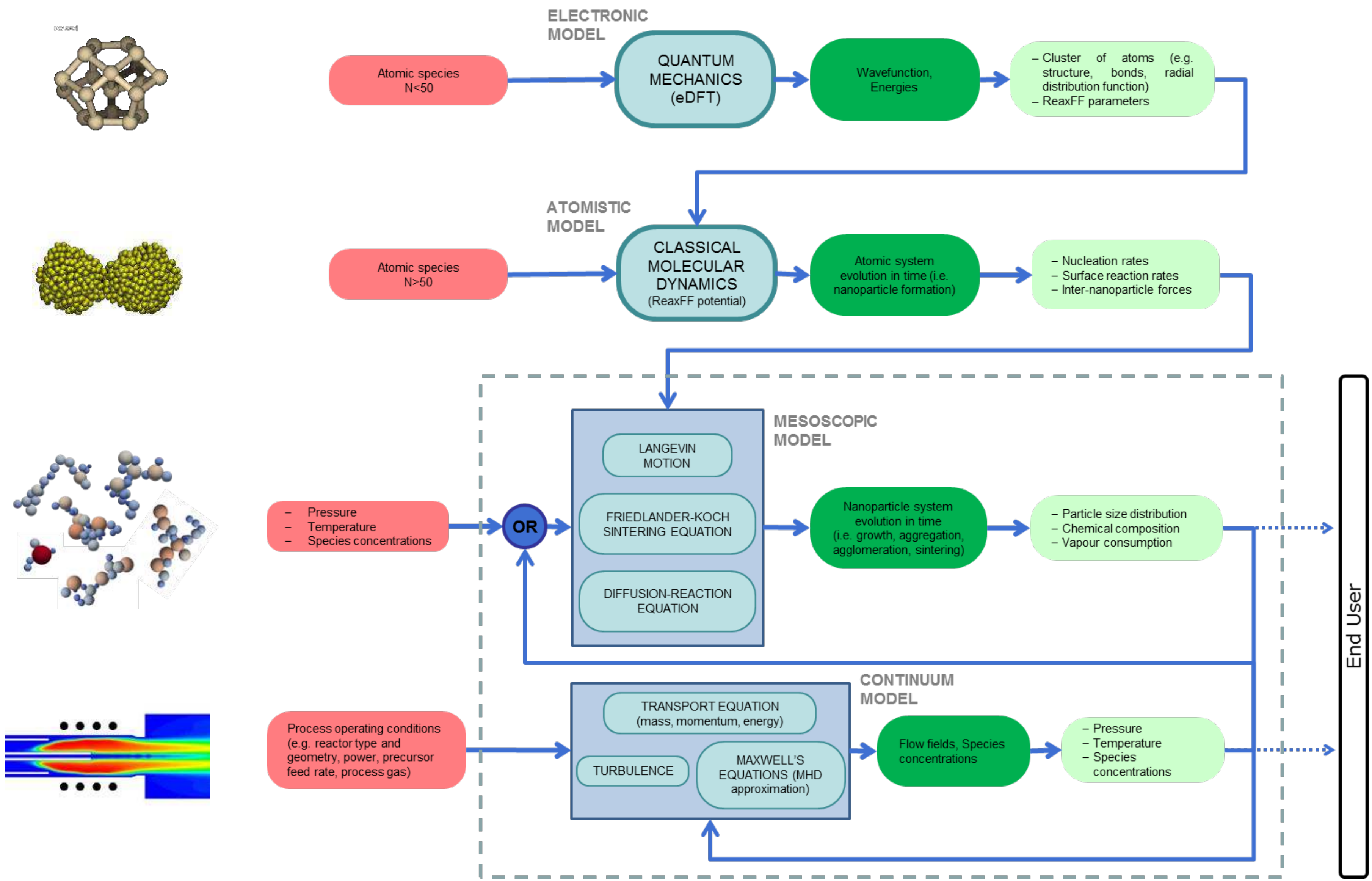
ALMA MATER STUDIORUM UNIVERSITÀ DI BOLOGNA



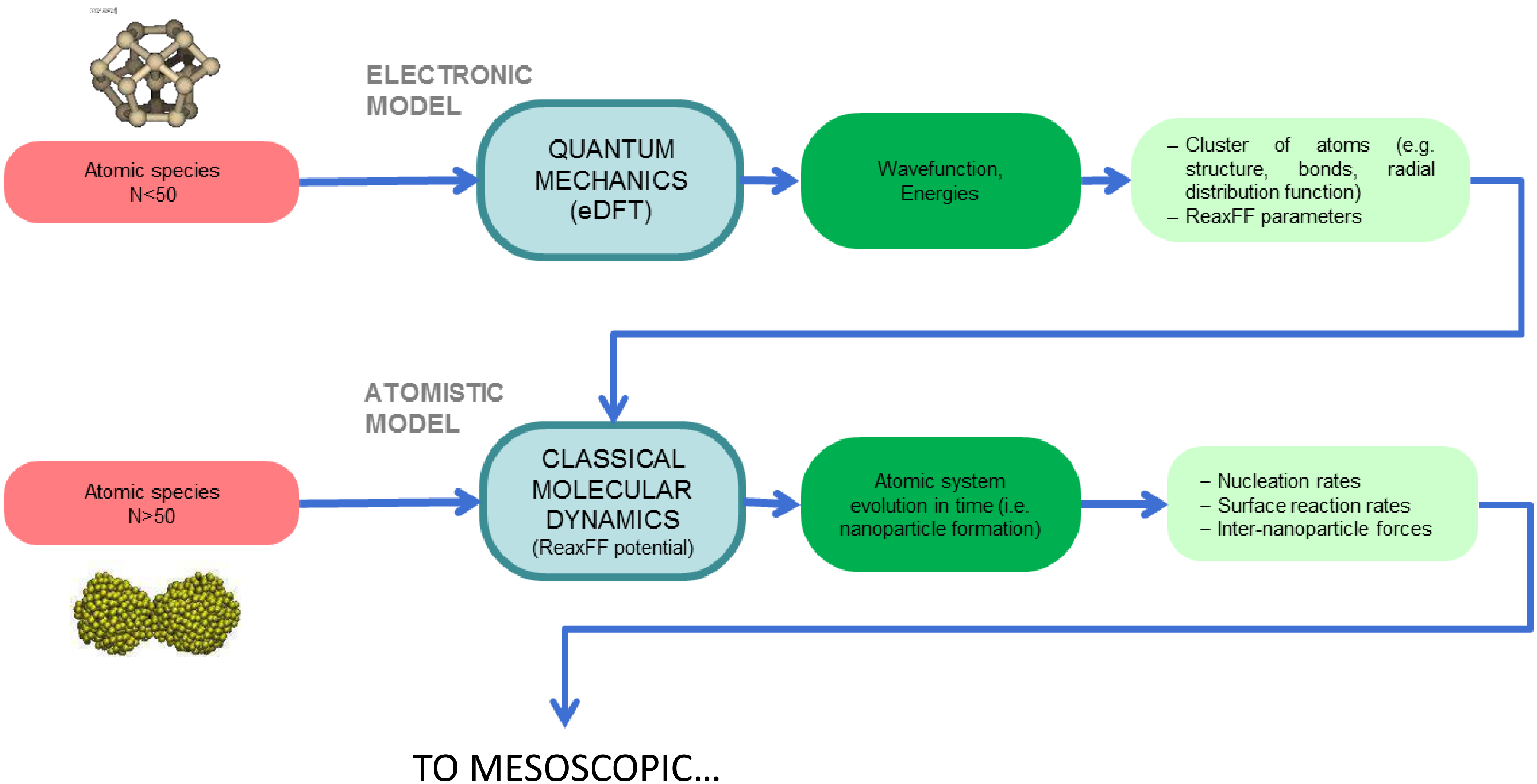

UNIVERSITÄT DUISBURG ESSEN Offen im Denken
UNIVERSITY OF CAMBRIDGE Chemical Engineering and Biotechnology
IPCF ISTITUTO PROCESSI CHIMICO-FISICI
umicore materials for a better life
CMCL Innovations

# USE CASE

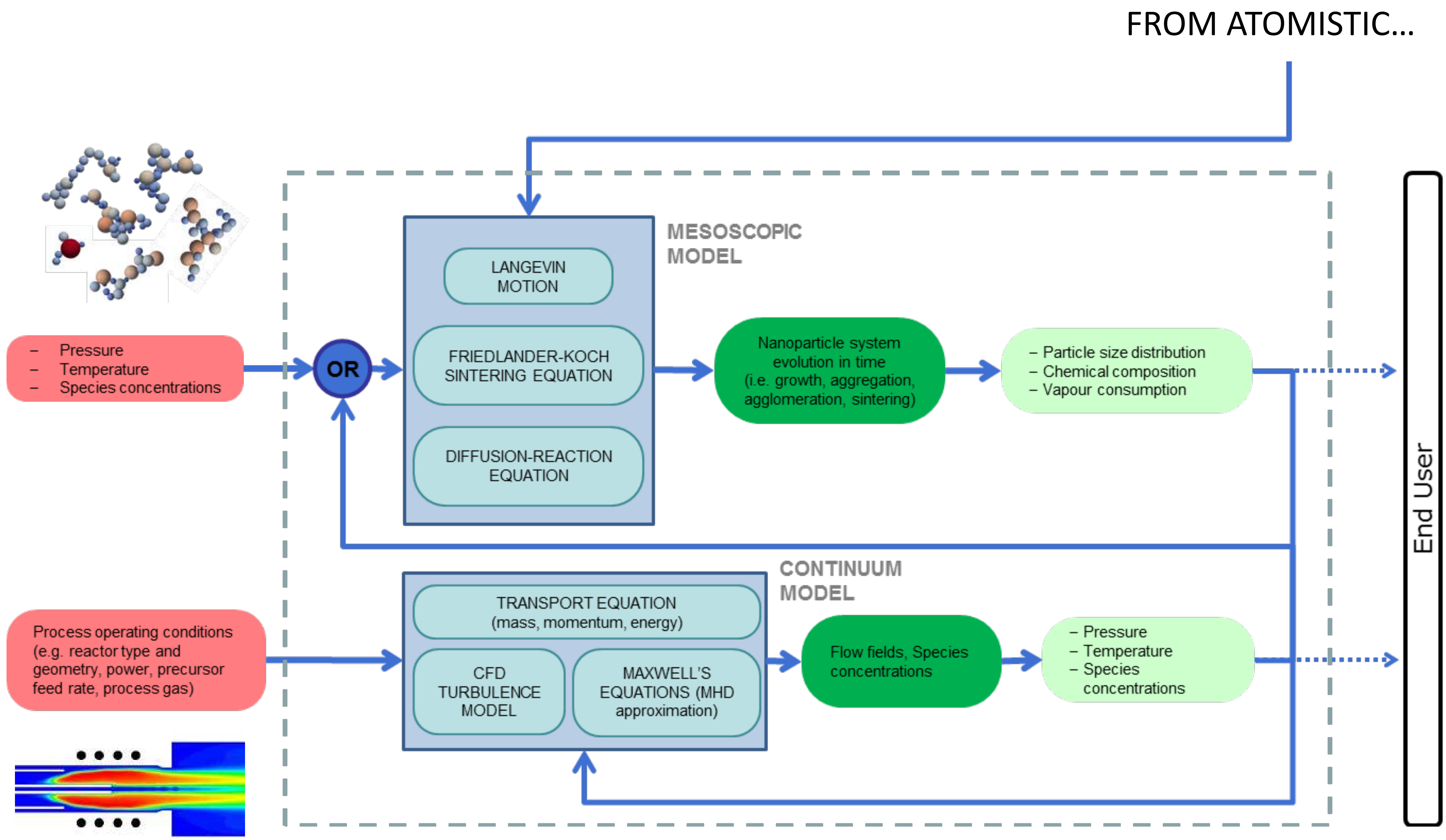
NanoDome



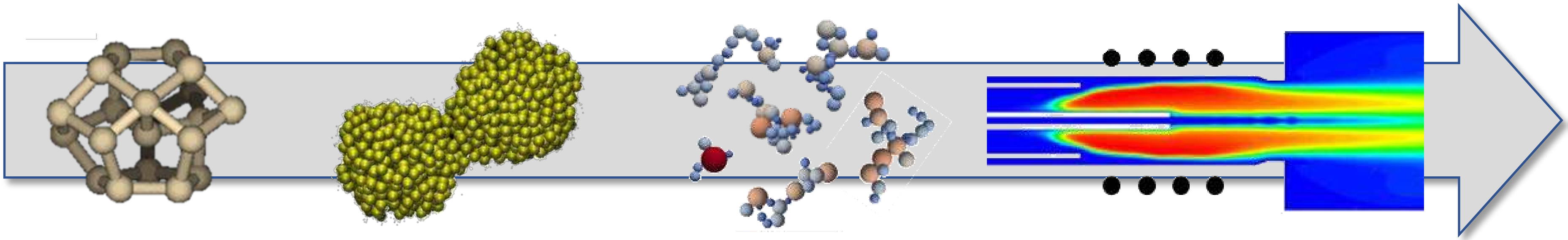
# USE CASE


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
TO MESOSCOPIC…

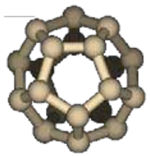
# USE CASE

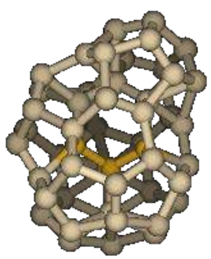

FROM ATOMISTIC…
MESOSCOPIC MODEL
LANGEVIN MOTION
FRIEDLANDER-KOCH SINTERING EQUATION
DIFFUSION-REACTION EQUATION
– Pressure
– Temperature
– Species concentrations
OR
Nanoparticle system evolution in time (i.e. growth, aggregation, agglomeration, sintering)
– Particle size distribution
– Chemical composition
– Vapour consumption
CONTINUUM MODEL
TRANSPORT EQUATION (mass, momentum, energy)
CFD TURBULENCE MODEL
MAXWELL'S EQUATIONS (MHD approximation)
Process operating conditions (e.g. reactor type and geometry, power, precursor feed rate, process gas)
Flow fields, Species concentrations
– Pressure
– Temperature
– Species concentrations
End User

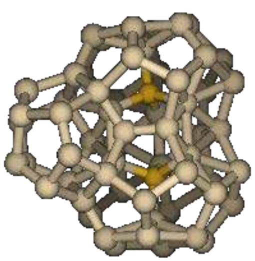
| OVERVIEW of the SIMULATION | | |
|---|---|---|
| **USER CASE** | Nanoparticle synthesis via gas phase condensation in industrial commercially-relevant processes. Prediction of the nanoparticle size distribution, morphology and internal composition via modelling of the gas phase condensation synthesis process, including homogeneous and heterogeneous nucleation, surface and internal chemical kinetics and composition, agglomeration, aggregation. Materials: Si, ZnO, $Al_2O_3$, Pt nanoparticles in $Ar/H_2/N_2/O_2$ atmospheres for synthesis processes in plasma, hot wall and flame reactors | |
| **CHAIN OF MODELS** | **MODEL 1** | Density Functional Theory (Electronic) |
| | **MODEL 2** | Classical Molecular Dynamics (Atomistic) |
| | **MODEL 3** | Coarse Grained Molecular Dynamics (Mesoscopic) |
| | **MODEL 4** | Fluid mechanics, Heat-Flow, Chemistry Reaction Model, Electromagnetism (Continuum) |
| | **DATA-BASED MODEL** | n.a. |
| **PUBLICATION PEER-REVIEWING THE DATA** | *n.a. (model is still in development)* | |
| **ACCESS CONDITIONS** | Electronic and Atomistic models are based on widely available commercial or open-source licenses packages, such as Quantum ESPRESSO, LAMMPS, ReaxFF, GROMACS, GARFFIELD. The mesoscopic model will be developed within the NanoDome project under open-source license. Continuum models are based on the commercial package ANSYS Fluent and on the open-source package OpenFOAM. Interfacing libraries and the material database for Si/Ar system will be open-source. Material database for reactive materials will be published under commercial license. | |
| **WORKFLOW AND ITS RATIONALE** | The CGMD model (mesoscopic) can fully describe a nanoparticle structure by predicting the growth mechanisms. Classical MD (atomistic) is needed to fill the unknown material relations for the nanoaprticle materials to be modelled, while DFT (electronic) is needed to increas the accuracy of existing interatomic potentials to be used by MD. A continuum description of the synthesis environment (the synthesis reactor) is needed to bring the model to an industrial user level. Linking/coupling between mesoscopic and continuum models makes these two models a single tool for the design of nanomaterial synthesis process. | |



# USE CASE – MODEL 1







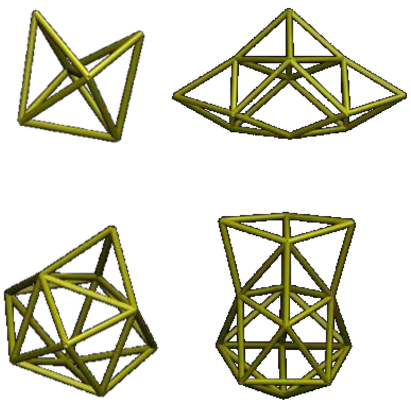
MODEL 1 (Electronic)

| | |
|---|---|
| **ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED** | |
| **ASPECT OF THE USER CASE TO BE SIMULATED** | Quantum calculations on small clusters: structural and static properties, molecular dynamics (finite temperature) for the optimization of the reactive force field, modelling of the very first stages of the nucleation processes, modelling of mutual interaction between clusters, benchmark for classical molecular dynamics. |
| **MATERIAL** | Atoms and small clusters with explicit description of electrons |
| **GEOMETRY** | Small clusters (less than 50 atoms) in a periodic box |
| **TIME LAPSE** | Below 1 ns |
| **MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS** | Density and concentration of species, constant volume or constant pressure |
| **PUBLICATIONS ON THIS DATA** | n.a. |

MODEL 1 (Electronic)

| | | |
|---|---|---|
| **MODEL EQUATION** | | |
| **MODEL TYPE AND NAME** | Density Functional Theory | |
| **MODEL ENTITY** | Electrons | |
| **MODEL PHYSICS EQUATIONS** | **EQUATION** | Schroedinger equation. Kohn–Sham equation |
| | **PHYSICAL QUANTITIES** | Wave function, electron density, total energy. |
| **MATERIAL RELATIONS** | **RELATION** | Local (Coulomb) and non-local (exchange) potential from electron density, and gradient of the electron density and pseudo potentials for the implicit core electron. |
| | **PHYSICAL QUANTITIES** | Density functionals, pseudopotentials, plane wave basis set. |
| **SIMULATED INPUT** | n.a. | |

# USE CASE – MODEL 1



**MODEL 1 (Electronic)**

| SOLVER AND TRANSLATION OF THE SPECIFICATIONS | | |
|---|---|---|
| NUMERICAL SOLVER | Self-consistent field (iterative approach) | |
| SOFTWARE TOOL | Quantum Espresso, CP2K, Dalton, Gamess | |
| TIME STEP | Femtoseconds for the molecular dynamics | |
| COMPUTATIONAL REPRESENTATION | PHYSICS EQUATION | Projection of differential equations on finite basis set |
| | MATERIAL RELATIONS | Hardcoded potentials. |
| | MATERIAL | Electrons are represented as material points,<br>Atoms are represented as ions implicitly including core electrons |
| COMPUTATIONAL BOUNDARY CONDITIONS | Cubic box with periodic boundary conditions. | |
| ADDITIONAL SOLVER PARAMETERS | *n.a.* | |

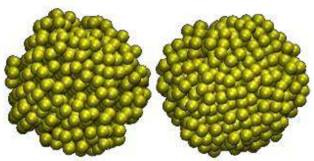
## ReaxFF

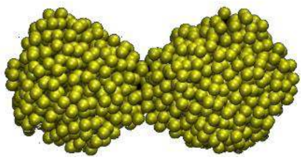
$$E_{system} = E_{bond} + E_{lp} + E_{over} + E_{under} + E_{val} + E_{pen} + E_{coa} + E_{C2} + E_{tors} + E_{conj} + E_{H-bond} + E_{vdWaals} + E_{Coulomb}$$

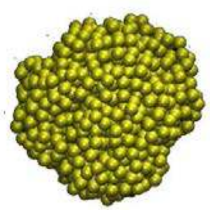
**MODEL 1 (Electronic)**

| POST PROCESSING | |
|---|---|
| THE PROCESSED OUTPUT | Cluster of atoms representation(e.g. structure, bonds, radial distribution function).<br>ReaxFF parameters for atomistic simulations. |
| METHODOLOGIES | Analysis, by visualization and computational tools, of geometrical structure, bonding environment, radial distribution functions etc. |
| MARGIN OF ERROR | The error depends on input parameters (density functionals, pseudopotentials, basis sets, size of the model system, time step and total simulation time) and is different for different physical properties: bonding distances and bonding angles (<5%), bonding energies (about 5%) |

# USE CASE – MODEL 2







**MODEL 2** (Atomistic)

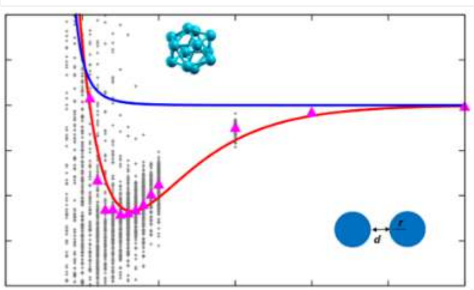
| **ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED** | |
|---|---|
| **ASPECT OF THE USER CASE TO BE SIMULATED** | Nucleation of atoms from gas phase to form primary nanoparticles and gas phase condensation on nanoparticle surface<br>Mutual interaction between nanoparticles (i.e. agglomeration, sintering) |
| **MATERIAL** | Atoms (atoms or molecules) in gas and condensed liquid/solid phase (nanoparticles) |
| **GEOMETRY** | Nanometre sized cubic box, representative a control volume of the reactor |
| **TIME LAPSE** | Microseconds. |
| **MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS** | Temperature time gradient (cooling), fixed external pressure, species concentration. |
| **PUBLICATIONS ON THIS DATA** | *n.a.* |

**MODEL 2** (Atomistic)

| **MODEL EQUATION** | | |
|---|---|---|
| **MODEL TYPE AND NAME** | Classical Molecular Dynamics | |
| **MODEL ENTITY** | Atoms | |
| **MODEL PHYSICS EQUATIONS** | **EQUATION** | Newton’s equation of motions. |
| | **PHYSICAL QUANTITIES** | Position, velocity, mass, interatomic potentials. |
| **MATERIAL RELATIONS** | **RELATION** | ReaxFF potential functions. |
| | **PHYSICAL QUANTITIES** | ReaxFF parameters includes:<br>• generic parameters<br>• atom parameters (per element)<br>• atom pairs/bond parameters (combination of two elements)<br>• angle parameters (combination of three elements)<br>• dihedrals (combination of four elements) |
| **SIMULATED INPUT** | ReaxFF parameters from DFT simulation. | |

# USE CASE – MODEL 2

NanoDome



PARAMETERS FOR NANOPARTICLES SINTERING TIME

$$\tau_S = A_{sint} d_p \exp(E_{sint}/T)$$

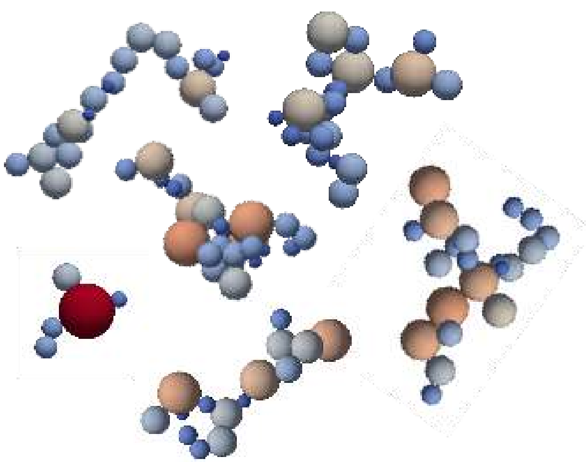
| MODEL 2 (Atomistic) | SOLVER AND TRANSLATION OF THE SPECIFICATIONS | | |
|---|---|---|---|
| | NUMERICAL SOLVER | | Velocity integrator schemes (e.g. Verlet Integration). |
| | SOFTWARE TOOL | | LAMMPS, http://lammps.sandia.gov<br>ReaxFF, http://www.scm.com/ReaxFF |
| | TIME STEP | | Femtoseconds |
| | COMPUTATIONAL REPRESENTATION | PHYSICS EQUATION | Discretization using e.g. Verlet-type scheme |
| | | MATERIAL RELATIONS | ReaxFF potential is hardcoded as function of atoms type and position. |
| | | MATERIAL | Atoms are represented are material points. |
| | COMPUTATIONAL BOUNDARY CONDITIONS | | Cubic box with periodic boundary conditions expressing infinite domain |
| | ADDITIONAL SOLVER PARAMETERS | | n.a. |

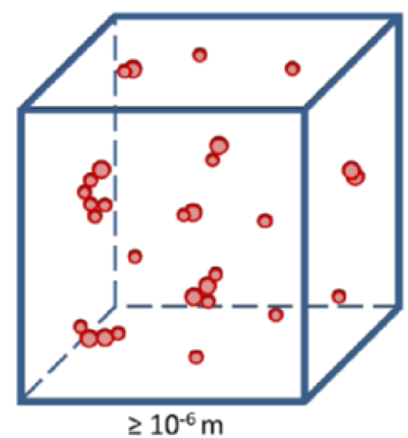
| MODEL 2 (Atomistic) | POST PROCESSING | |
|---|---|---|
| | THE PROCESSED OUTPUT | Interparticle potentials, sintering time and nucleation rates for nanoparticles (i.e. beads) |
| | METHODOLOGIES | Mapping matrix from a set of atomic coordinates to a unique nanoparticle configuration in the mesoscopic system by means of an atom-atom connection criterion.<br>Iterative Boltzmann conversion and/or force mapping algorithm to define CG energy functions (i.e. interparticle potentials) from the atomistic energy function. |
| | MARGIN OF ERROR | Accuracy of ReaxFF parameters and fitting (~8%)<br>Multiparticles interactions are often neglected in favour of binary interaction.<br>Application on limited time and domain and to one mechanisms at time (i.e. sintering, nucleation). |

# USE CASE – MODEL 3

NanoDome

| **MODEL 3** (Mesoscopic) | **ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED** | |
|---|---|---|
| | **ASPECT OF THE USER CASE TO BE SIMULATED** | Nanoparticle growth inside a meso-scale control volume and evolution of the nanoparticle ensemble including agglomeration, sintering and chemical reactions in plasma, hot wall and flame nanoparticle synthesis processes. |
| | **MATERIAL** | Nanoparticles of Si, ZnO, Al3O3, Pt in Ar/H2/N2/O2 atmospheres |
| | **GEOMETRY** | Micrometer sized cubic box representative of the interior of the reactor |
| | **TIME LAPSE** | Milliseconds. |
| | **MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS** | Temperature time gradient (cooling), fixed external pressure. |
| | **PUBLICATIONS ON THIS DATA** | *n.a.* |





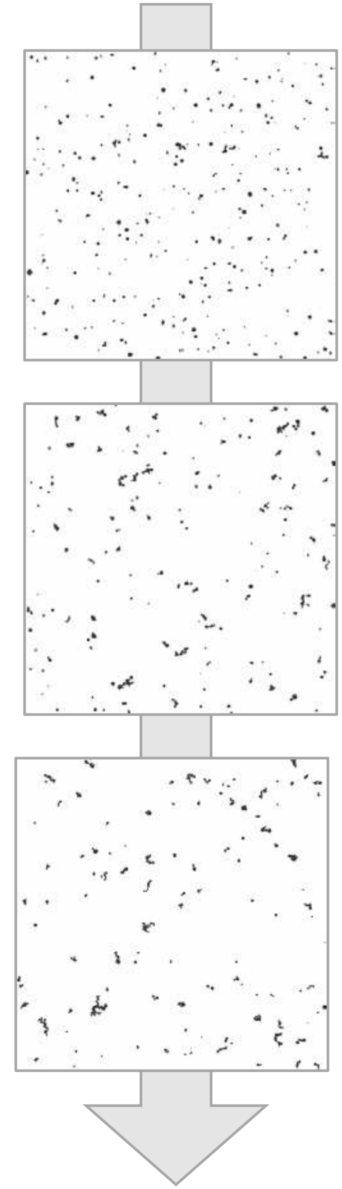

*Meso-scale model simulation box.*

# USE CASE – MODEL 3

NanoDome

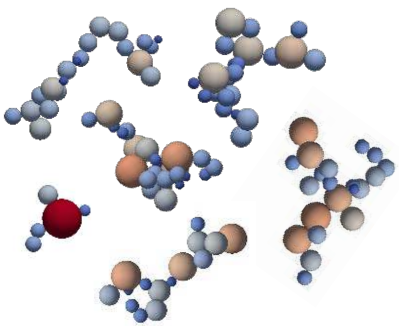
**MODEL 3** (Mesoscopic)

| MODEL EQUATION | | |
|---|---|---|
| MODEL TYPE AND NAME | Coarse Grained Molecular Dynamics | |
| MODEL ENTITY | Nanoparticles (beads) | |
| MODEL PHYSICS EQUATIONS | EQUATION | 1. Langevin's equation of motions for single particles and particle aggregates: $$m_i \frac{d^2\mathbf{x}_i}{dt^2} = \mathbf{F}_i(t) - m_i \gamma \mathbf{v}_i + \beta(t)$$ 2. Modified Koch and Friedlander equation for sintering process: $$\frac{dA}{dt} = -\frac{1}{\tau}(A - A_f)$$ 3. Diffusion-reaction equation (conservation of mass) for internal nanoparticle concentration profile: $$\frac{\partial n_X}{\partial t} - D_X \Delta n_X = -k n_A n_B$$ |
| | PHYSICAL QUANTITIES | 1. Position ***x***, velocity ***v***, mass *m* and inter-particle forces ***F***.<br>2. Particle area *A*, coalescence area $A_f$ and sintering time $\tau$.<br>3. Species radial distribution for each nanoparticle $n_X$ (X = A,B), diffusion coefficient $D_X$ and reaction rate constant *k*. |
| MATERIAL RELATIONS | RELATION | 1. Nanoparticle interaction forces $\boldsymbol{F}_i$ between grains (nanoparticles) based on van der Waals-like potentials: $\boldsymbol{F}_i = -\nabla V(r)$<br>2. Friction coefficient *g* on a spherical particle<br>a. Stokes law $\gamma = 6\pi\eta R_i$<br>b. Epstein relation $\gamma = \frac{4}{3}\delta\pi R_i^2 \frac{p}{k_B T} m_g \langle v_g \rangle$<br>3. Semi-empirical relation predicting particle sintering time $t_s$ as function of: $$\tau_S = \tau_S(p_i, p_j) = A_{sint} d_p \exp(E_{sint}/T)$$ 4. Nucleation and growth rates from Classical Nucleation Theory |
| | PHYSICAL QUANTITIES | 1. Nanoparticle interaction potential *V(r)*<br>2. Particle radius $R_i$, gas molecule mass $m_g$, average gas velocity $<v_g>$, gas pressure and temperature *p* and *T*.<br>3. Material dependant properties ($A_{sint}$, $E_{sint}$), temperature *T* and particles diameter $d_p$.<br>4. Pressure, temperature and material properties of the condensing species (i.e. surface tension, bulk density, saturation pressure) |
| SIMULATED INPUT | Interparticle potentials, sintering time and nucleation rates for nanoparticles from atomistic simulations. Gas phase composition, temperature and pressure from user of from coupled/linked continuum models. | |

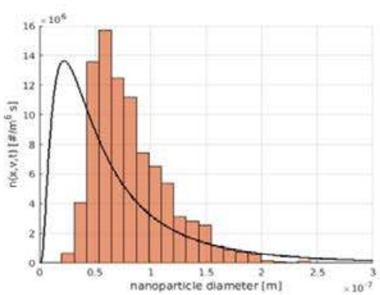


# USE CASE – MODEL 3

NanoDome



| MODEL 3 (Mesoscopic) | | | |
|---|---|---|---|
| **Solver and Translation of the Specifications** | | | |
| **Numerical Solver** | | Time integration via symplectic splitting method for Langevin dynamics. ODE solver for chemical kinetics equations. PDE solver for particle concentration profile. The equations are solved coupled together using operator splitting technique (loose coupling). | |
| **Software Tool** | | In project developed, Open Source. | |
| **Time Step** | | Nanoseconds. | |
| **Computational Representation** | **Physics Equation** | Verlet discretization. Explicit time discretization for ODE. Spatial discretization for PDE. | |
| | **Material Relations** | Hardcoded functions. | |
| | **Material** | Primary particles as spherical mass objects (beads) with variable species composition. Nanoparticles as rigid body aggregates of primary particles. | |
| **Computational Boundary Conditions** | | Periodic boundary conditions. | |
| **Additional Solver Parameters** | | n.a. | |

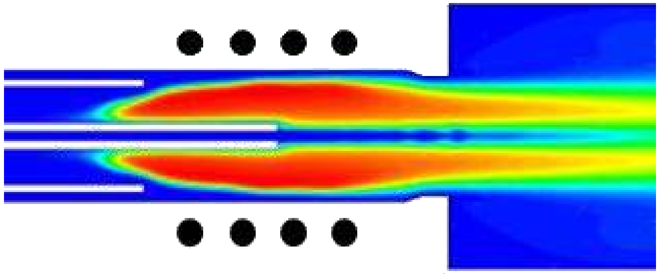



| MODEL 3 (Mesoscopic) | |
|---|---|
| **Post Processing** | |
| **The Processed Output** | Finite volume. Precursor vapour consumption for continuum model coupling. |
| **Methodologies** | Simple integration on the particle set or particle counting. Aggregates properties (e.g. fractal dimension, mass, diameter) obtained by looping on particles structures. |
| **Margin of Error** | Errors related to particle idealization (e.g. spherical shape), chemical reduction, interparticle forces, sintering mechanism and limited number of particles in the mesoscopic ensemble. Using temperature and composition data from a continuum fluid model streamline means that nanoparticle diffusion between continuum regions is neglected. |

# USE CASE – MODEL 4

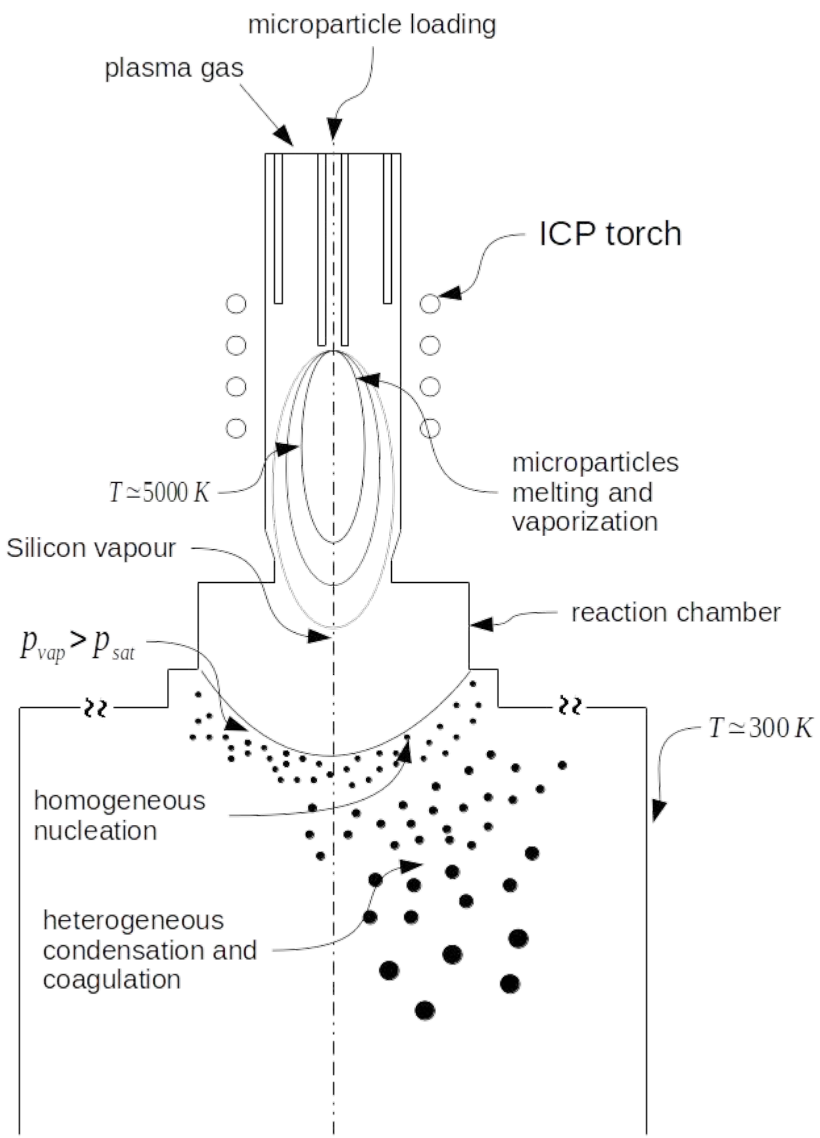
NanoDome

| MODEL 4 (Continuum) | ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED | |
|---|---|---|
| | **ASPECT OF THE USER CASE TO BE SIMULATED** | Flow characteristics (e.g. velocity, temperature, species concentration) in a gas phase reactor (plasma, flame and hot wall reactors). |
| | **MATERIAL** | Gaseous, liquid or solid precursors.<br>Si, ZnO, $Al_2O_3$, Pt nanoparticle synthesis in $Ar/H_2/N_2/O_2$ atmospheres. |
| | **GEOMETRY** | Chemical synthesis reactor. Centimetres. |
| | **TIME LAPSE** | Seconds. |
| | **MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS** | Gas phase condensation synthesis reactor: plasma, flame or hot-wall. |
| | **PUBLICATION** | n.a. |



# USE CASE – MODEL 4

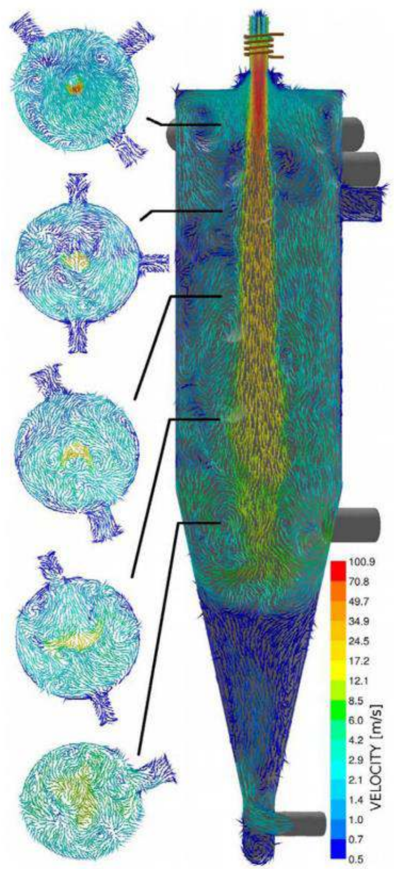
NanoDome




| 2 | GENERIC PHYSICS OF THE MODEL EQUATION | | |
|---|---|---|---|
| MODEL 4 (Continuum) | MODEL TYPE AND NAME | | Fluid Dynamics |
| | MODEL ENTITY | | Finite volumes. |
| | MODEL PHYSICS/ CHEMISTRY EQUATION | EQUATION | 1. Generic transport conservation equation for:<br>$$\frac{\partial \rho\phi}{\partial t} + \nabla\cdot(\rho\vec{u}\phi) = \nabla\cdot\vec{q_\phi} + S_\phi$$<br>a. mass (species)<br>b. momentum (Navier-Stokes)<br>c. energy<br>2. Turbulence models (Reynolds Averaged Navier Stokes and/or LES)<br>3. Electromagnetic field equations for plasmas (Maxwell's equation under usual Magneto Hydro Dynamics simplifications) |
| | | PHYSICAL QUANTITIES | 1. The general conservation equation is written for:<br>*a.* $\phi = Y_i$ : $\boldsymbol{q}_i$ diffusion flux for species $i$, $S_i$ source terms due to chemical reactions and nanoparticle nucleation (from the meso-scale model).<br>*b.* $\phi = \boldsymbol{u}$ : $\boldsymbol{q}_u$ momentum flux, $\boldsymbol{S}_u$ Lorentz forces (plasma)<br>*c.* $\phi = h$ : $\boldsymbol{q}_h$ heat flux, $S_h$ source terms due to chemical reactions or Joule heating (plasma)<br>with density $\rho$ and velocity $\boldsymbol{u}$.<br>2. Turbulence parameters (e.g. turbulence kinetic energy $k$)<br>3. Vector $\boldsymbol{A}$ and scalar $V$ potential (plasma) |
| | MATERIALS RELATION 1 | EQUATION | 1. Constitutive equations for:<br>a. $\boldsymbol{q}_i$ using multicomponent (or binary) diffusion, $S_i$ from Arrhenius based equations for reaction rates.<br>b. $\boldsymbol{q}_u$ assuming Newtonian linear relationship between stress and deformation tensors (Navier-Stokes equation)<br>c. $\boldsymbol{q}_h$ heat flux in a multispecies environment.<br>2. Turbulence:<br>a. $\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$ for Standard k-ε RANS and standard closure coefficients<br>b. subgrid scale model for LES<br>3. Simplified Ohm's law for current density $\boldsymbol{j}$ (thermal plasmas): $\boldsymbol{j} = \sigma\boldsymbol{E}$ |
| | | PHYSICAL QUANTITIES/ DESCRIPTORS | 1. Descriptors for each equation are:<br>a. Pre-exponential factor and activation energy for rate constant calculation for each reaction of the reduced chemical kinetic model and species diffusion coefficients (including thermal diffusion)<br>b. Fluid transport properties (e.g. viscosity)<br>c. Fluid transport and thermodynamic properties (e.g. thermal conductivity, specific heat).<br>2. Closure coefficients from the specific model used (e.g. k-e, RSM, Smagorinsky)<br>3. $\sigma$ electrical conductivity and $\boldsymbol{E}$ electric field (plasma) |
| | PUBLICATION | | |

# USE CASE – MODEL 4

NanoDome




MODEL 4 (Continuum)

| SOLVER AND TRANSLATION OF THE SPECIFICATIONS | | |
|---|---|---|
| NUMERICAL SOLVER | | Finite volumes. Equations are usually solved with loose coupling (segregated solvers) due to the high non-linearity of the coefficients and source terms. |
| SOFTWARE TOOL | | ANSYS Fluent (commercial), OpenFOAM (open source) |
| TIME STEP | | Steady state, or time dependent for LES simulations ($10^{-5}$ – $10^{-4}$) s |
| COMPUTATIONAL REPRESENTATION | PHYSICS EQUATION | Finite volume discretization of the transport equation. Vector and scalar potential form of the Maxwell's equation discretized in a finite volume framework. |
| | MATERIAL RELATIONS | Hardcoded as function of discretized space-time variables (e.g. reactions rates, heat flux and N-S stress tensor contitutive equations and turbulence closures relations for LES and RANS) |
| | MATERIAL | Species densities control volume-wise. |
| COMPUTATIONAL BOUNDARY CONDITIONS | | Gas/precursors feeding rates and operating pressure.<br>Generator power (for plasma sources) |
| ADDITIONAL SOLVER PARAMETERS | | n.a. |

MODEL 4 (Continuum)

| POST PROCESSING | |
|---|---|
| THE PROCESSED OUTPUT | Flow fields, temperature fields, species concentrations calculated via postprocessing for the larger (macroscopic) finite volumes (gas phase). |
| METHODOLOGIES | Position in time (i.e. streamline), temperature in time, species concentration in time calculated for single finite volume. |
| MARGIN OF ERROR | For plasma simulations, the margin of error in the predicted temperature field is expected to stay below 10% (SIMBA project results).<br>Errors related to the limited amount of streamline used for mesoscopic models, chemical reduction, turbulence models. |

# METADATA

**Metadata** are defined as data and schema that describe and give information about a data describing a specific domain knowledge.

MODA
structure of knowledge

as top-level METADATA SCHEMA

describes all aspects of a material modelling and metadata can be built on that basis by making use of the **semantic rules** – i.e., relations - defined by the **common vocabulary**

**MODA** can be used to lay out the **top-level (upper) ontology of material modelling**, and allow harvesting specific **vocabularies** and bridging over vocabulary barriers used in different communities by harvesting **semantic** communalities from different MODA describing essentially the same model schemes.

- **exchange of information** between materials modelling codes
- putting data in a form that allows models to **properly recognize** it along with its 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)

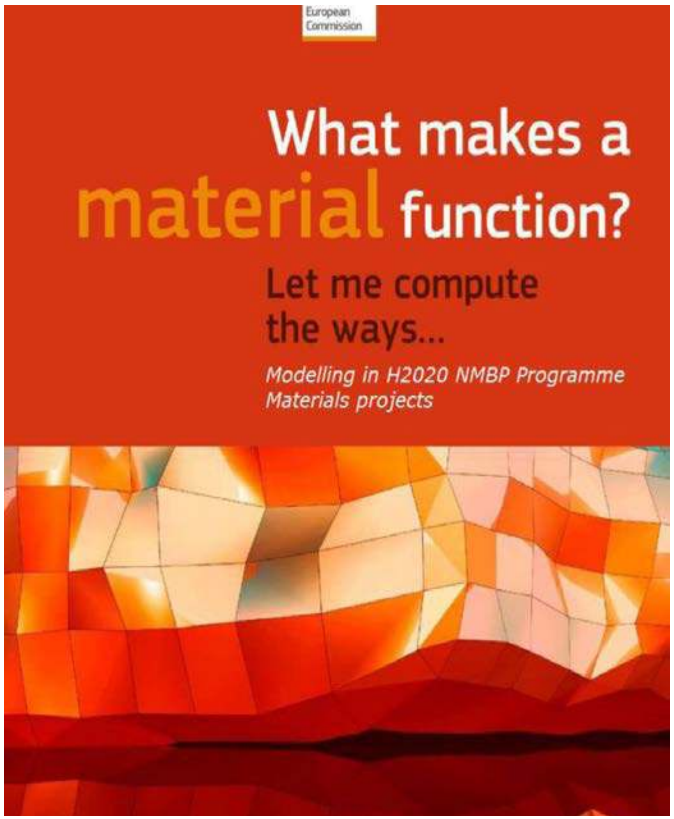
# EMMC PLANS FOR THE NEAR FUTURE

- Provide a first set of **standard PE and MR** for the **most common models**, so that every applicant **will not reinvent the wheel**
- Provide a **selected small set** of **MODA examples** for **basic user cases** for different fields of applications to be used as reference point (MODA examples are already published in the RoMM IV for each H2020 project, but is not easy to navigate through them)
- Distinguish between **free text field entries** (e.g. description) and **fixed options** (e.g. model entities)
- **MODA online form** for easy compilation, catalogue and formatting.

MORE SUGGESTIONS ARE WELCOME!

# ACKNOWLEDGEMENTS

YOU CAN FIND ALL THESE THINGS
EXTENSIVELY EXPLAINED
IN THE RoMM VI




***Modelling in H2020 LEIT-NMBP Programme Materials and Nanotechnology projects***

# 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/