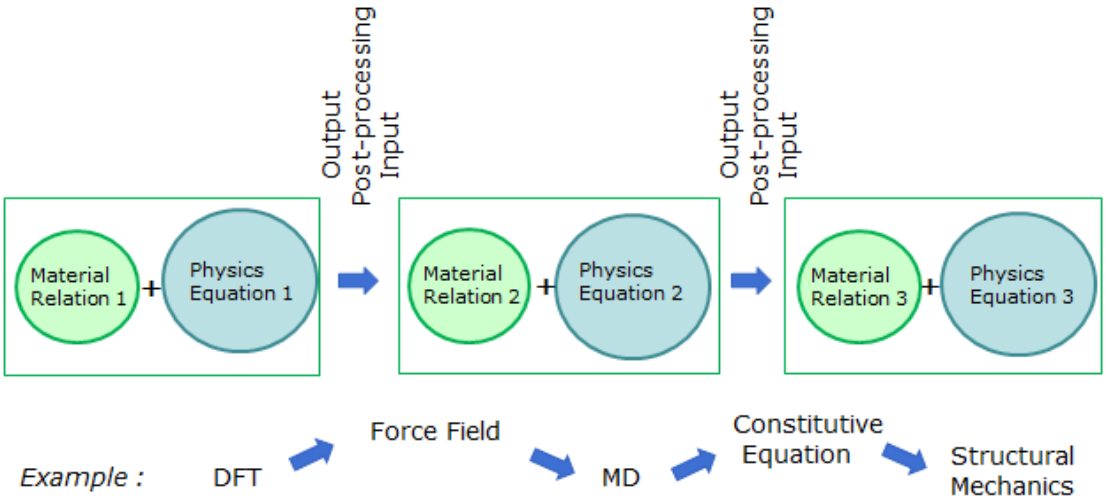
Summary of the new Modelling Vocabulary

These two pages attempts to summarise in a concise manner the Modelling Vocabulary.

What are Models? What are Simulations?

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

> The "*physics or chemistry equations*" describe the behaviour of electrons, atoms, particles or finite volumes (the model entities). The physics or chemistry equations are generic and applicable to many situations.



> Physics or chemistry equations need to be complemented with information on the application (material). This information is given in relations applicable to a certain class of materials. These relations close the physics/chemistry equations and make them solvable. In many fields, especially in the continuum model world, they are called constitutive equations, but in order to harmonise all fields we opt for the name "*material relations*".

Materials Modelling is the establishing of governing equations (**PE** and/or **MR**) for physical or chemical quantities. These governing equations contain the key assumptions of the model. Modelling does not include fitting parameters in existing governing equations to (simulated or experimental) data.

Simulation software is a computational code, which solves the governing equations by numerical methods and requires information about the application (boundary and initial conditions)

➔ Models are the Governing Equations of the physical and chemical entities, not the codes or simulation software. A code can contain the implementation of one or several models (toolkit/framework/workbench).

Material Model Types

A new way of building an overview of materials models consists in classifying the models according to the physics and chemistry included. Classification can be done via the ***entity*** whose behaviour is described by the model, nl: *electrons*, *atoms*, *nanoparticles/beads/grains* and *continuum in finite volumes/elements.*

> The model approximations might use concepts like density of entities (like e.g. in electronic or atomistic DFT), collective spectral behaviour of entities (e.g. in phonon models describing heat in atomic crystals), but this does not influence the classification.

The four natural categories consist of three **discrete** types and one **continuum** type of models:

Method	**Entity whose behaviour is described**	**Number of units**	**Length scale**	**Time scale**
Electronic models	electron	10-100	0.1 - 1 nm	-
Atomistic models	atom	10^2 - 10^9	0.1 – 100 nm	fs - µs
Mesoscopic models	nanoparticle, beads, mesoscopic particles, grains	10^6-unlimited	100 nm - mm	ms - s
Mesoscopic magnetism models			1 nm - 100 mm	1 ps - 1000 ns
Continuum approaches	continuum finite volumes	unlimited	nm-m	s - ks

Models are strictly classified according to the entity described by the model and not according to the size of the application or system.

The reason for this is that classifying models according to the size (length -scale) of their application, rather than their entities, does not convey any meaningful information on the nature and hence the accuracy of the models. For example, a microstructure domain of some nano meters length can be modelled by considering either electrons, atoms, grains or finite volumes/elements. Thus calling the model after the application size "a mesoscale model" does not reveal enough information for material scientiststhat want to know whether the phenomena are described by the Schrödinger equation, Newton dynamics, conservation equations, or other physics equations.

Electronic models

These models describe the behaviour of electrons using quantum mechanical physics equations that calculate electronic structures from *first principles*. The physics equation is the Schrödinger equation with a set of approximations.

List of electronic Models

- **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 and projector-augmented waves
  - 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
  - 1.4.2 Percolation models
- **1.5 Statistical electron spin transport model**

Atomistic models:

These models describe the behaviour of atoms. They ignore the electronic degrees of freedom and use mechanics (forces and potentials) to describe the behaviour of atoms.

List of atomistic models

- **2.1 Classical Density Functional Theory and 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**
  - 2.5.1 Deterministic spin models
  - 2.5.2 Langevin dynamics model for magnetic spin systems
- **2.6 Statistical transport model at atomistic level**
- **2.7 Atomistic phonon models** (Boltzmann Transport Equation)

Mesoscopic (particle) models:

These models describe the behaviour of (part of) molecules, nanoparticles, bead, mesoscopic particles or grains, while what happens inside such an entity is considered to be frozen.

At the supra-atomic scale, uninteresting or fast details of the atomic motions can be averaged out or replaced by stochastic terms, and the mesoscopic models concentrate on essential motions of entities that are formed from more than one atom. The models describe the interactions between the beads.

List of mesoscopic models:

Continuum models:

These models describe the behaviour of a continuum entity called finite volume or finite element. At this level material is assumed to be continuously distributed throughout its volume. Continuum models disregard the discrete particle-based structures and smaller details.

List of continuum models:

Interoperability of models (multi-scaling) and databases

Linking models is running different models consecutively (sequential modelling).
Coupling models is running different models concurrently (concurrent modelling).

A major issue in linking models is transfer of data from one model to another. The post-processing (reduction, extraction) of model output turns it into input for the next model in the form of values for parameters or new materials relations. Post-processing can be purely mathematical fitting data when the value of a parameter in a known materials relation is calculated. Sometimes physics is included to verify that the averaged field still makes sense. Post-processing also involves physics, when the modellers are looking for new materials relation. Then they have to have an idea (assumption) for what physics relation they are looking. And this relation is then proven by the data. In continuum modelling, often the results of continuum models applied at meso-scale (nm) are fed into the continuum model applied at macro-scale model (μm) in the form of constitutive equations – which in the language of the brochure are called material relations - or as boundary conditions. The establishment of such constitutive equations represents a big challenge in contemporary modelling. Another example of finding a new template materials relation is finding a force field including extra physics/chemistry processes.

Finally, last but not least, often not only models are to be connected but integration of experimental data should also be done in a clever way.

Solvers

Solvers are used to solve the physics/chemistry equation. In the Review there is a strict separation between the two concepts "solver" and "model". For example, smoothed particle hydrodynamics (SPH) is a solver (used to discretise the fluid dynamics model equations) and not a model. Kinetic Monte Carlo is a way to solve mechanics equations. FEM is a solver and contains no physics information.

Solvers sometimes use concepts like "fictitious particles" but these are not to be confused with the entities whose behaviour is to be described.