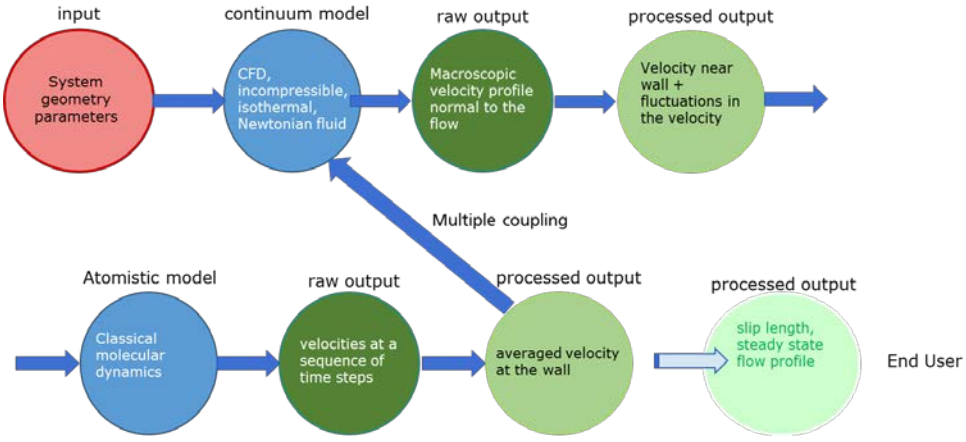
Elements in materials modelling

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	*Velocity flow profile in a micro or nano channels taking into account the effects of micro or nano structure of the channel walls on the flow pattern*	
2	CHAIN OF MODELS	MODEL 1	*Continuum, CFD model*
		MODEL 2	*Atomistic, Molecular Dynamics*
		...	...
3	PUBLICATION ON THE SIMULATION	*In Preparation.*	
4	ACCESS CONDITIONS	*Free and open code, see http://github.com/simphony*	



SimPhoNy

Workflow

CFD is used to describe flow in a pipe. MD is used to refine what happens at the walls. This MODA is for a simple example where the wall structure is translationally invariant, so we pick just one place to describe it atomistically. The flow velocity change at the wall due to the nano and micro structure is calculated by averaging over a number of time steps of the simulation (up to few pico seconds). The main assumption is that this time interval is small enough that no change can be observed on the macroscale (in the continuum model). This is moved back to the continuum model as a wall boundary condition on the velocity.

Each model used in a simulation can be documented in three chapters:

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

This processes the output of one simulation into input for the next simulation.

Please use the following four tables to document each "simulation with one model".
Coupled models can be written up collectively in one set of four tables.

Elements in the simulation with CFD

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	*Velocity profile for liquid flowing in a straight rectangular nano and micro structured channel.*
1.2	MATERIAL	*The channel walls are assumed to be made of glass or polystyrene, and the fluid is water based.*
1.3	GEOMETRY	*A long rectangular channel, about 1 cm long, and 50μm up to 1000μm in width. Water enters from the right and exits from a left inlet.*
1.4	TIME LAPSE	*up to 10s of seconds*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*There is a constant pressure difference imposed externally across the channel.*
1.6	PUBLICATION ON THIS ONE SIMULATION	*Publication documenting **the simulation** with this single model (if available and if not included in the overall publication). In Preparation*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Continuum Fluid Mechanics, Fluid Dynamics*	
2.1	MODEL ENTITY	*finite volumes*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	*Name and description and mathematical form of the PEs* 1. *The Navier-Stokes(N-S) Equation for incompressible isothermal fluid:* $\rho\left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\right] = -\nabla p + \mu\nabla^2\boldsymbol{v} + \boldsymbol{f}$ 2. *Mass conservation equation for incompressible fluid (liquid):* $\nabla\cdot(\boldsymbol{v}) = 0$...
		Physical quantities for each equation	*Please name the physics quantities (parameters (constants, matrices) and variables that appear in these equations e.g. wave function, Hamiltonian, spin, velocity, external force).* 1. N-S equation: ρ: *density*, $\boldsymbol{v}$: *velocity*, p: *pressure*, μ: *dynamic viscosity*, $\boldsymbol{f}$: *external body forces (e.g., gravitation)* 2. Mass conservation equation: ρ: *density*, $\boldsymbol{v}$: *velocity* *In both equations, the independent variables are time t, and position* $\boldsymbol{r}$.
MATERIALS RELATIONS		**MR Equations**	*Strictly speaking, there are no further materials relations requiring additional equations, since the assumption of*

		incompressible, isothermal and Newtonian Fluid viscosity model have already been "consumed" in the general Cauchy relations to obtain the N-S equation. In this case the viscosity and density are just properties of the material (constants).
	Physical quantities/ descriptors for each MR	
2.4	**SIMULATED INPUT**	*After an initial iteration, the MD simulation gives the velocity at the wall as boundary conditions. It is assumed that the velocity is translationally invariant along the walls in steady state.*

This part 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	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	*Finite Volume Method*	
3.2	**SOFTWARE TOOL**	*SimPhoNy using the OpenFOAM wrapper*	
3.3	**TIME STEP**	*Dynamic, set by solver to keep accuracy reasonably sufficient, typical values 1e-5 seconds*	
3.4	**COMPUTATIONAL REPRESENTATION** *Refers to how your computational solver represents the material, properties, equation variables,*	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*The computational domain is discretised on a structured mesh. Each mesh element has cell centres and 6 faces. The integral form of the PE from section 1, the MR and the material is written up for a finite volume mesh. Cell centres and faces have the following properties:* *Cells contain the v and p fields. Faces contain fluxes.* *Computationally, each equation is represented by a standard data schema as described in the SimPhoNy CDUS and CUBA: CUBA.CFD_MODEL, CUBA.INCOMPRESSIBLE_MODEL, CUBA.ISOTHERMAL_MODEL* *The computational Mesh is also described using CUBA and the CUDS schema: each mesh element has a data property with key-value sets, the keys are standard CUBA.PRESSURE, CUBA.VELOCITY. The material properties such as density and viscosity are described according to the CUDS schema by standard keywords: CUBA.DENSITY and CUBA.VISCOSITY*
		BOUNDARY CONDITIONS	*Mesh elements that belong to each boundary (inlet, outlet and channel/pipe walls) can be identified on each of the variables (pressure and velocity) in the PE. Specific boundary conditions are specified to* ***translate*** *the physics boundary conditions and process conditions in section 1 for the walls and the inlet and outlet.* • *For Velocity:* a. *on walls: no-slip (fixed velocity, coming from the atomistic model)* b. *on inlet: pressure inlet velocity, as pressure is fixed and known at inlet, the velocity is evaluated from the flux normal to the inlet* c. *on outlet: zero gradient on U* • *For Pressure:* a. *on channel walls: adjust the pressure gradient so that the boundary flux matches the velocity boundary condition (in OF fixedFluxPressure).* b. *on inlet: fixed value* c. *on outlet: fixed value* *In SimPhoNy this is done by marking the mesh elements that are on boundaries and associating them with the proper boundary conditions using CUBA and CUDS.*

		ADDITIONAL SOLVER PARAMETERS	*Maximum Courant Number, Mesh cell size.*

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 circles in the workflow picture.
This output is processed by a post processor in order to calculate values for physics variables for larger entities that can be input to the next model or that are the final output of the total simulation.
The physics used to do this calculation is to be documented.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*velocities and positions of the atoms near the wall*
4.2	METHODOLOGIES	*Statistical velocity variations are added which fulfil the classical Maxwell-Boltzmann distribution*
4.3	MARGIN OF ERROR	*If the boundary conditions are chosen correctly, the velocity is accurate at the macroscopic level, with a margin of up to 5%.*

Elements in the simulation with MD

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	*The effect of nano and micro structure in the wall on the velocity of a fluid near a wall*
1.2	MATERIAL	*The wall and fluid are as above, with the same friction.*
1.3	GEOMETRY	*A small box representing the fluid near a small area of the wall (height is 1/10th of the pipe diameter, length is long enough to obtain a stable flow))*
1.4	TIME LAPSE	*up to few 10s of picoseconds*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*There is an initial flow profile driving the flow through the channel*
1.6	PUBLICATION ON THIS ONE SIMULATION	*Publication documenting **the simulation** with this single model (if available and if not included in the overall publication).*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Atomistic, Molecular Dynamics*	
2.1	MODEL ENTITY	*Atoms*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	*Newton equations of motion for a set of N interacting particles (atoms)* $m_i\ddot{r}_i = f_i$, *for i=1,2,…N* $f_i = \nabla_{r_i} V(r_1, r_2, \dots)$
		Physical quantities for each equation	• m_i: *mass of an atom,* $\boldsymbol{r}_i$: *position of an atom,* $\boldsymbol{f}_i$: *the force on an atom, which in principle is a result of the interaction with all other atoms and external forces which is given by the potential energy* $V(r_i)$. 1. *The independent variables are time t, and position* $\boldsymbol{r}$.
MATERIALS RELATIONS		**MR Equations**	1. *A simple shifted Lennard-Jones Pair potential with a cut-off distance* • $u^{LJ}(r_i, r_j) = 4\epsilon[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}$ $r \le r_c$ • 0 for $r > r_c$
		Physical quantities/ descriptors for each MR	1. u^{LJ} *is the potential energy between two atoms at positions* r_i *and* r_j. r_{ij} *is the distance between the atoms,* σ *is the van der Walls radius (related to the effective size of each atom), and* ϵ *is the energy well depth.* r_c *is the cut-off distance.*
2.4	SIMULATED INPUT	*The velocity field coming from the macroscopic simulation is used as initial condition for the velocities of the atoms. Statistical velocity variations are added which fulfil the classical Maxwell-Boltzmann distribution*	

This part 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	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	*Finite Different (Verlet)*	
3.2	SOFTWARE TOOL	*SimPhoNy with the LAMMPS wrapper*	
3.3	TIME STEP	*1 femto second*	
3.4	COMPUTATIONAL REPRESENTATION *Refers to how your computational solver represents the material, properties, equation variables,*	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*The walls are made of fixed (fictitious) atoms while the fluid is represented by a number of interacting atoms. The rheology of the atomistically represented fluid is chosen to be the same as that of the continuum (macroscopic) model. Atoms are represented by their positions (points)* • *The physical variables, velocity, mass and acceleration are given at each point.* • *The atoms are confined to a box (in this case rectangular).* *The walls are represented by fixed atoms that interact with the liquid (using the same LJ potential). The walls are structured* *Computationally in SimPhoNy the model equations are identified by a CUBA.MOLECULAR_DYNAMICS keyword.*
		BOUNDARY CONDITIONS	*Periodic boundary conditions are assumed along the flow direction and fixed boundaries normal to the flow. These are identified in SimPhoNy by a CUBA.PERIODIC_BOUNDARY_CONDITIONS keyword*
		ADDITIONAL SOLVER PARAMETERS	*Pure internal numerical solver details that are often set* 1. *Specific tolerances* 2. *Cut-offs, convergence criteria* 3. *Integrator options*

Post processing

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This output is processed by a post processor in order to calculate values for physics variables for larger entities that can be input to the next model or that are the final output of the total simulation.
The physics used to do this calculation is to be documented.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*Flow velocity change at the wall in finite volumes.*
4.2	METHODOLOGIES	*Sampling and averaging of the velocity profile on the atomistic level is performed using the SimPhoNy developed wrappers and post/pre-processors.*
4.3	MARGIN OF ERROR	*At this level, the LJ pair potentials are known to be notorious as they do not specifically describe the liquid state sufficiently. Hence there are large errors to be expected, up to 20% in velocity.*