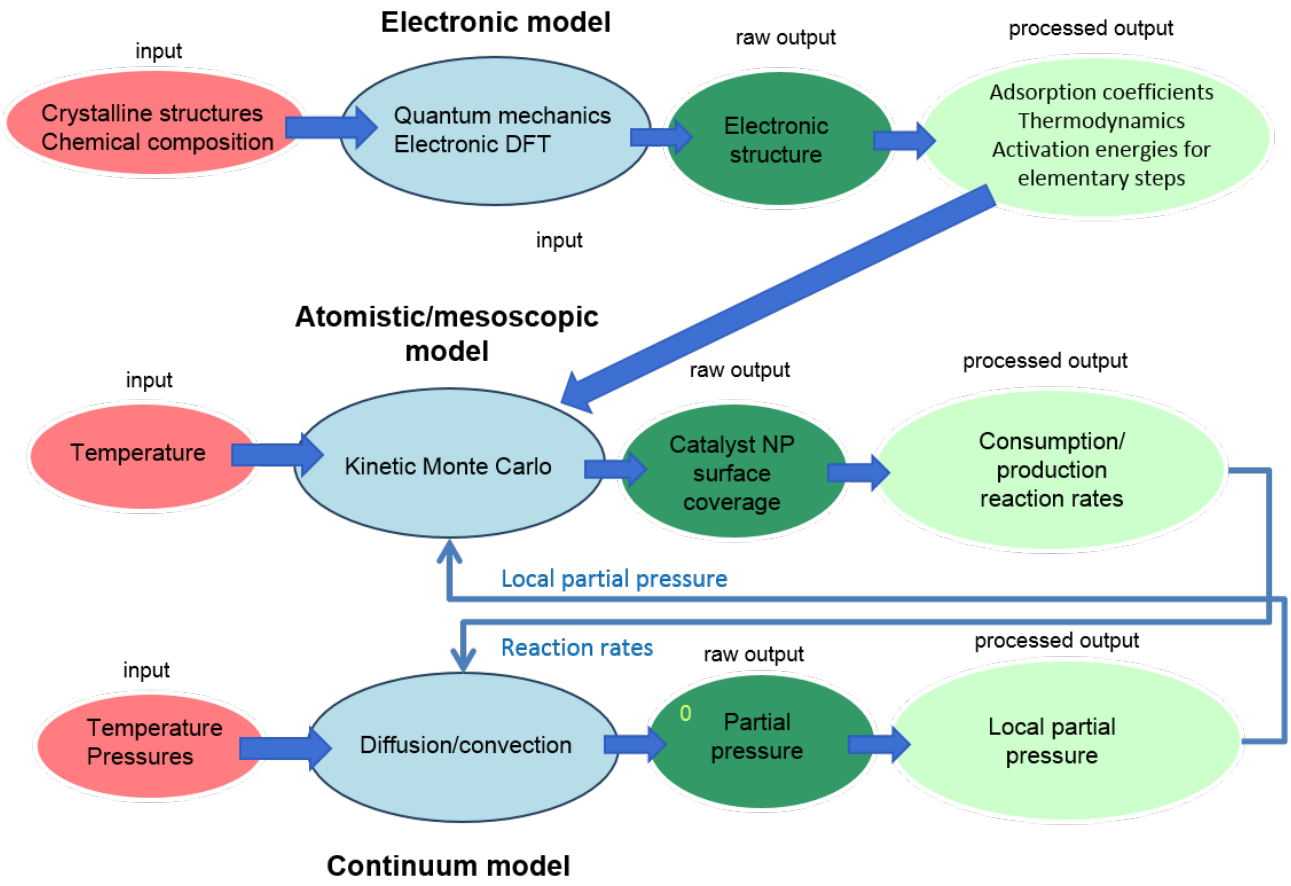
Elements in materials modelling

Each simulation will have its own 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.

Note: in the following only the chemical reactor case is being illustrated.
A second user case, the lithium ion battery, is simulated analogously.

THE SIMULATION GENERAL DESCRIPTION			
1	USER CASE	*Elementary kinetics and reactants/products transport processes in porous carbonaceous materials supporting catalyst nanoparticles.*	
2	CHAIN OF MODELS	MODEL 1	*Electronic structure of the catalyst materials via Density Functional Theory.*
		MODEL 2	*Reaction kinetics on catalyst nano-particles surfaces via Kinetic Monte Carlo (coupled to **Model 3**)*
		MODEL 3	*Diffusion/convection transport of reactants/products in the full porous materials via continuum approach (coupled to **Model 2**)*
3	PUBLICATION	*J. Catal. 285, 273-284 (2012),* *Nature Chem. 4, 739-745 (2012),* *J. Phys. Chem. C 118, 19023-19031 (2014).* *M.A. Quiroga, K. Malek, A.A. Franco, J. Electrochem. Soc., **163** (2) (2016) F59.* *M.A. Quiroga, A.A. Franco, J. Electrochem. Soc., **162** (7) (2015) E73.* *A.A. Franco, M.L. Doublet, W. Bessler, Eds., "Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage", Springer, UK (2015).*	
4	ACCESS CONDITIONS	*The electronic structure calculated data will be available through the ioChem-BD.org platform that has been established at ICIQ by the Proof-of-Concept BigData4Cat* *The coupled continuum/KMC calculations on the full porous materials will be done by using the in-house code MS LIBER-T at CNRS developed since more than 14 years* *(see: http://modeling-electrochemistry.com/ms-liber-t/).*	



Workflow example of chain of three models

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

Between each two simulations or models, some post/pre-processing may take place. This processes the output of one simulation into input for the next simulation.

MODEL 1: DFT

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*Surface process at the elementary step levels*
	MATERIAL	*Metals acting as catalyst.*
1.3	GEOMETRY	*The systems will be clusters, surface, interface and bulk with up to 200 atoms.*
1.4	TIME LAPSE	*N/A*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*bulk of catalyst material and interface between catalyst material and gas , catalyst nanoparticle.*
1.6	PUBLICATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Ab initio quantum mechanical models : (Electronic) Quantum Density Functional Theory*	
2.1	MODEL ENTITY	*Electrons*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	Schrödinger equation
		Physical quantities for each equation	Energies, electron density, spin density, wave function
MATERIALS RELATIONS		**Equations**	1. Kohn-Sham 2. Bloch theorem 3. Hellman-Feymann forces (local energy minimisation procedure to explore the potential energy surface) 4. Transition state theory 5. Themodynamics
		Physical quantities/ descriptors for each MR	1. Electron Density 2. Electronic band structure, Phonon band structure, Density of States 3. Equilibrium structures 4. Activation energy barriers

		5. Reaction energies , adsorption energies
2.4	**SIMULATED INPUT**	Chemical Compositions / Guessed structures
2.5	**PUBLICATION**	*Publically available standard DFT Density Functional Theory: A Practical Introduction D. Scholl, J. A. Steckel*

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**	*Kohn-Sham-DFT*	
3.2	**SOFTWARE TOOL**	*VASP and Gaussian*	
3.3	**TIME STEP**	*Not applicable*	
3.4	**COMPUTATIONAL REPRESENTATION** *Density, electron number, geometries*	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*Written up for the electron density*
		BOUNDARY CONDITIONS	*Periodic boundary conditions*
		ADDITIONAL SOLVER PARAMETERS	*Pure internal numerical solver details that are often set* 1. *Specific tolerances* 2. *Cut-offs, convergence criteria* 3. *Integrator options* *All of them employed by default in the programs*
3.5	**PUBLICATION**		

Post processing

The "raw output" calculated by the model for the model entities is contained in the metadata above (physics quantity in the PE). This output is processed by a post processor in order to calculate values for physics variables for larger entities.
When this post-processed output is used in a next model, a pre-processor might be used.

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	*Adsorption energies, species involved in the surface diffusion, activation energies for the elementary reactions* *Destination entity: atoms and molecules for the atomistic/mesoscopic KMC (**Model 2**)*
4.2	**METHODOLOGIES**	*Processing through standard simulation packages,*
4.3	**MARGIN OF ERROR**	*0.4 eV for adsorption energies* *0.1 eV for the kinetic barriers* *Of the elementary processes*

MODEL 2: Atomistic and mesoscopic kMC

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED		*Operation solving chemical reactions on catalyst nanoparticles with particular local partial pressures*
	MATERIAL		*Catalyst nanoparticles (Pt, Pd)*
1.3	GEOMETRY		*Three-dimensional (shape of the nanoparticles)*
1.4	TIME LAPSE		*Nanoseconds to days (temporal multi-scale)*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS		*Local partial pressures of reactants and products, temperature,*
1.6	PUBLICATION		
2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	MODEL TYPE AND NAME		*KMC part of MS LIBER-T*
2.1	MODEL ENTITY		*Atoms, molecules*
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	*Markovian equations (Kinetic Monte Carlo approach within the Variable Step Size Method).*
		Physical quantities for each equation	*Chemical potentials, fluxes, surface concentrations.*
MATERIALS RELATIONS		**Equations**	*Probability functions.*
		Physical quantities/ descriptors for each MR	*Kinetic parameters, surface diffusion coefficients, defects surface concentrations*
2.4	SIMULATED INPUT		*local partial pressure (calculated by **Model 3**)*
2.5	PUBLICATION		

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		*Variable Step Size Method*
3.2	SOFTWARE TOOL		*MS LIBER-T / MESSI: http://modeling-electrochemistry.com/ms-liber-t/*
3.3	TIME STEP		*Variable time step*
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*The solver represents the materials as a discrete collection of atoms/molecules.*

		BOUNDARY CONDITIONS	*Periodic boundary conditions*
		ADDITIONAL SOLVER PARAMETERS	*Specific tolerances* *Cut-offs, convergence criteria* *Integrators options*
3.5	**PUBLICATION**		

Post processing

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When this post-processed output is used in a next model, a pre-processor might be used.

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	*Reaction (production/consumption) rates calculated for finite volume, the whole bulk? as inputs for the **Model 3***
4.2	**METHODOLOGIES**	*Volume averaging*
4.3	**MARGIN OF ERROR**	*N/A*

MODEL 3: CONTINUUM: Diffusion and convection

Elements in the simulation with one single materials model from the chain

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*transport by diffusion/convention in the porous component for specific local reaction rates*
1.2	MATERIAL	*catalytic reactor: carbon, catalyst (Pt, Pd)*
1.3	GEOMETRY	*catalytic reactor (thickness = to be defined from the project future specifications)*
1.4	TIME LAPSE	*Nanoseconds to days (temporal multi-scale)*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*Inlet/outlet reactants/products pressures, temperature*
1.6	PUBLICATION	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Continuum Diffusion and Convection*	
2.1	MODEL ENTITY	*finite volumes*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	*Set of 20 (in average) coupled Partial Differential Equations and Ordinary Differential Equations formulated within the non-equilibrium thermodynamics approach (mass, energy conservation equations).*
		Physical quantities for each equation	*Chemical potentials, molar fluxes, intermediate reaction species volume concentrations.*
MATERIALS RELATIONS		**Equations**	*Constitutive equations for the reactions and transport coefficients(*
		Physical quantities/ descriptors for each MR	*Diffusion coefficients, pore size distributions, particle size distributions*
2.4	SIMULATED INPUT	*Reaction rates (Source terms) calculated by the KMC (discrete) part in MS LIBER-T (**Model 2**).*	
2.5	PUBLICATION		

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	*Finite Volume Method*	
3.2	SOFTWARE TOOL	*MS LIBER-T: http://modeling-electrochemistry.com/ms-liber-t/*	
3.3	TIME STEP	*Variable time step*	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*The solver represents the composite electrodes as a continuum meshed in finite volumes*
		BOUNDARY CONDITIONS	*Newman, Dirichlet and mixed boundary conditions depending on the components (e.g. electrode, separator...) and systems being simulated.*
		ADDITIONAL SOLVER PARAMETERS	*Specific tolerances* *Cut-offs, convergence criteria* *Integrators options*
3.5	PUBLICATION		

Post processing

The “raw output” calculated by the model for the model entities is contained in the metadata above (physics quantity in the PE) . This output is processed by a post processor in order to calculate values for physics variables for larger entities.
When this post-processed output is used in a next model, a pre-processor might be used.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*Outlet reactants/products composition, outlet pressure which enters in the MR (kinetic rate expressions) in the kMC*
4.2	METHODOLOGIES	*Averaging*
4.3	MARGIN OF ERROR	*N/A*