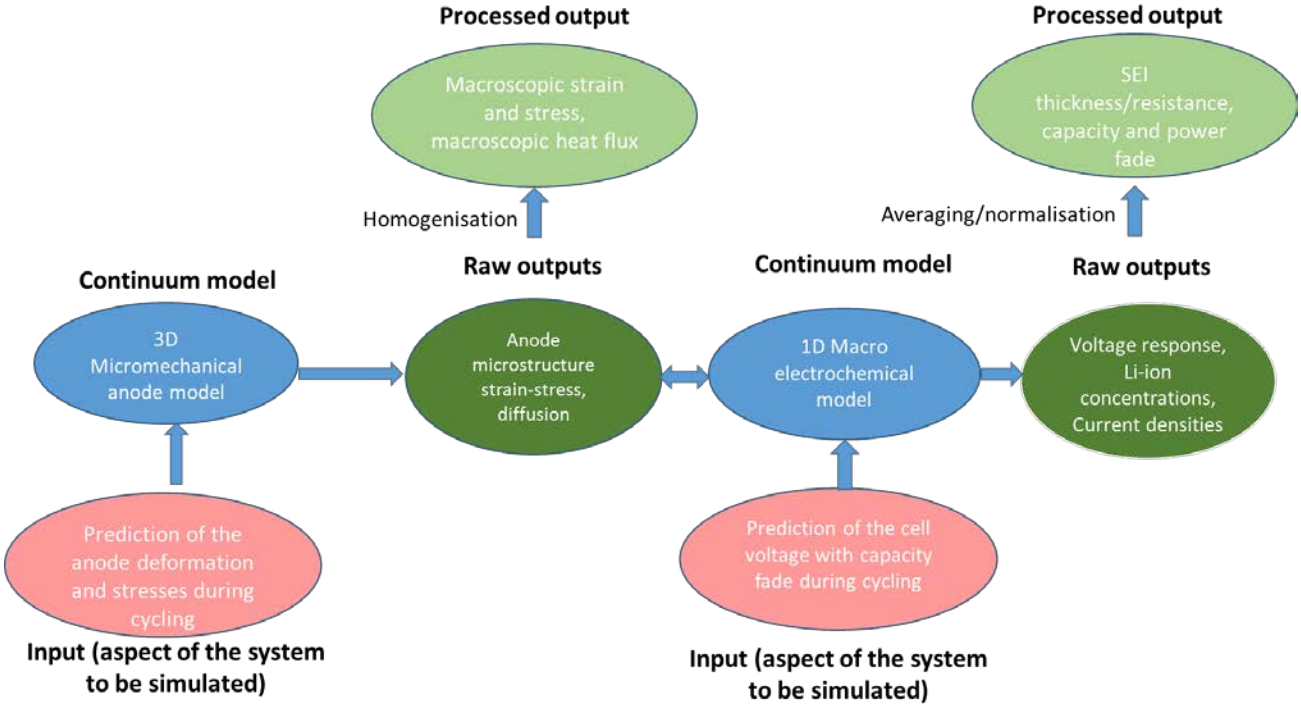
Elements in materials modelling in SINTBAT

THE SIMULATION GENERAL DESCRIPTION			
1	USER CASE	Prediction of the large strain deformation and associated stresses within the anode during cycling. To predict the voltage response of the Li-ion Si anode cell with capacity fade due to SEI growth during cycling	
2	CHAIN OF MODELS	MODEL 1	3D Micromechanical model based on the Representative Volume Element (RVE) concept
		MODEL 2	1D Macro Electrochemical model
3	PUBLICATION	Not yet available	
4	ACCESS CONDITIONS	The models and post processed data will be distributed among project partners. They will be owned by WMG (Nanocomposites Modelling Group and Energy and Electrical Systems Group) at the University of Warwick. External users may be given access upon contacting the owners.	



Workflow of the continuum models

Elements in the simulation of Model 1: 3D Micromechanical model

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	A 3D micromechanical model for prediction of the deformation and stresses during lithiation/delithiation of the anode will be developed. The micromechanical model will be based on the RVE concept to reflect the in-situ behaviour of the anode. The large deformation behaviour will be driven by the response of Si particles undergoing large volumetric deformations. The medium between Si particles will be modelled as an effective nonlinear material governed by the response of binder material. The strains/stresses will be predicted both at the micromechanical level (raw data) and macroscopic level (post-processed data) using nonlinear computational homogenisation.
1.2	MATERIAL	Si particles, effective matrix
1.3	GEOMETRY	RVE
1.4	TIME LAPSE	From seconds to hours
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Lithium ion concentration, mechanical constraints
1.6	PUBLICATION	Not yet available

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum model. 3D Micromechanical model	
2.1	MODEL ENTITY	Finite volumes/elements	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	1. Stress-strain-like law 2. Fick's-like law
		Physical quantities for each equation	1. Stresses, strains 2. Concentration, fluxes
MATERIALS RELATIONS		**Equations**	1. Strain energy function 2. Fick's-like law
		Physical quantities/ descriptors for each MR	1. Material constants: stress-strain tangents, cross-link density 2. Diffusivity
2.4	PUBLICATION	Not available	

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	FE	
3.2	SOFTWARE TOOL	ABAQUS	
3.4	TIME STEP	Unclear	
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	PDEs
		MATERIAL RELATIONS	Stress-strain, Fick's-like law
		MATERIAL	Microstructure of the anode will be represented as a composite made of Si particles embedded in an effective matrix, with a possible interphase layer around Si particles
		BOUNDARY CONDITIONS	Li ion concentration, mechanical constrains (translational degrees of freedom)
		ADDITIONAL SOLVER PARAMETERS	Relevant parameters governing an iterative-incremental Newton-Raphson-like solution scheme
3.6	PUBLICATION	Not yet available	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Finite volumes/elements and RVE
4.2	METHODOLOGIES	Macroscopic strain and stress, macroscopic diffusion flux using computational homogenisation
4.3	MARGIN OF ERROR	Statistical evaluation of the mean and standard error will be evaluated by considering various RVE ensembles

Elements in the simulation of Model 2: 1D Macro Electrochemical model

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	To predict the voltage response of the Li-ion Si anode cell with capacity fade due to SEI growth during cycling
1.2	MATERIAL	Current collectors, electrode pair, separator and electrolyte
1.3	GEOMETRY	A 1D simplified representation of the current collectors, electrode pair, separator and electrolyte ~ 100 microns
1.4	TIME LAPSE	Seconds-hours
1.6	PUBLICATION	Upon project start

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum model. 1D Macro electrochemical model	
2.1	MODEL ENTITY	Finite volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE'S	**Equations**	1. Current density for intercalation and for SEI side reaction 2. Mass conservation in electrolyte and solid phase 3. Charge conservation in electrolyte and solid phase
		Physical quantities for each equation	1. Specific surface area, volume fractions, SEI conductivity 2. Diffusion coefficients, particle size 3. Solid and electrolyte conductivities
2.4	PUBLICATION	Upon project start	

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	Implicit TDMA	
3.2	SOFTWARE TOOL	Fortran/Matlab	
3.4	TIME STEP		
3.5	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION	PDE
		BOUNDARY CONDITIONS	Mostly Newman type, BC of solid phase potential (charge conservation) is governed applied cell charging-discharging current.
3.6	PUBLICATION	Upon project start	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	SEI thickness/resistance, capacity and power fade
4.2	METHODOLOGIES	Averaging/normalisations and solving a differential equation relating SEI thickness to rate of reaction
4.3	MARGIN OF ERROR	