MODA
Modelling DAta providing a description
for *self-heating of carbon fiber reinforced composite by Joule Effect*
simulated in project *MASTRO*

OVERVIEW of the SIMULATION			
1	**USER CASE**	The user wants to simulate the self-heating functionality of a percolator consisting of a conductive network shaped by nano-fillers reinforced with Carbon Fibers. In this case both nanofillers and fibers are conductive elements of the system. Self- heating is based on Joule Effect of the composite material filled with electrical conductive nanomaterial and coming from the carbon fibers.	
2	**CHAIN OF MODELS**	**MODEL 1**	Mesoscopic Model: Coarse Grained Molecular Dynamics to calculate chemical morphology of the material and its percolation threshold.
		MODEL 2	Continuum Electricity model for Percolation applied to a Resistor Network The result is post processed into generated heat. Equations: Tunneling Probability, Circuit Equation, Ohm Equation, Power Equation
		MODEL 3	Continuum Model: Tightly coupled electro-thermal model describing the joule effect applied to nm scale.
		MODEL 4	Continuum Model: Tightly coupled electro-thermal model describing the joule effect applied to cm scale.
3	**PUBLICATION PEER-REVIEWING THE DATA**	-	
4	**ACCESS CONDITIONS**	Model 1: inhouse Software OCCAM developed at UNISA will be used Model 2 : inhouse Ancillary code developed in UNISA in the OCCAM package Model 3, 4: not decided yet. Commercial FEM software can be used (COMSOL or ABAQUS). The choice of an open-source software is also possible to facilitate transfer to partner Link : In-house tools will developed to transfer the output at each step of the workflow	

MODA

Simulation with MODEL 1 – Mesocale GCMD

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Self-Assembly of a Structures of CNTs inside the dispersing matrix (resin or thermoplastic polymer)
1.2	MATERIAL	Thermoplastic Polymer or resin filled with CNTs
1.3	GEOMETRY	 A snapshot of a typical geometry obtained from simulation of self-assembly of CNTs in a polymeric matrix
1.4	TIME LAPSE	milliseconds
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Pressure, ambient temperature.
1.6	PUBLICATION ON THIS DATA	No publication yet

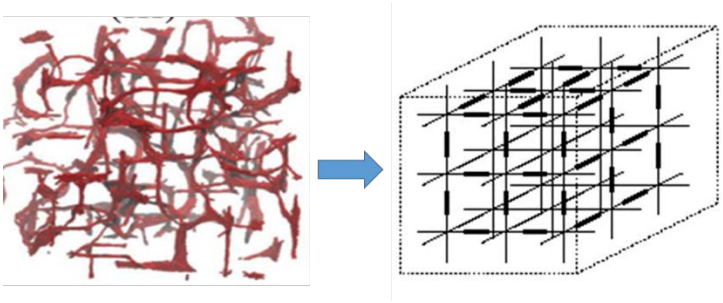
2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Mesoscopic Model: CG Molecular Dynamics with modified Thermostating scheme (	
2.1	MODEL ENTITY	Particles (atoms or effective beads grouping several atoms)	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Newton equations of motion, Thermostat (usually a constant temperature)is modified A particle, with a given probability, is subjected to random collision. The probability of collision is $$P(t) = \Gamma \Delta t$$ At each particle a random number between 0 and 1 is assigned. If this random number is smaller than $\Gamma \Delta t$ the velocity of the particle is reset. The velocity to be reset is taken from a Gaussian distribution around the set Temperature. The set Temperature, is fixed according to the position of the particle from the conditions imposed

			by models 2 and 4. In this thermostatting scheme the CGMD is divided into grid regions (cells), and the temperature of each cell is assigned according to the average kinetic energy of the atoms within the cell. On the top of this, new temperatures for each cell are then calculated stepwise concurrent with the MD simulation 2 numerically solving the continuum heat equation: $$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial r^2} + Q$$ *T* =temperature coming from the MD simulation of Model 1, *D*=thermal diffusivity *Q*= heat generated by power equation inside the grid region Particles velocities of in cells are scaled to match the numerical solution of the continuum heat equation above.
		Physical quantities	Main equation: Particle positions, particle masses, forces, particle velocities thermostat formula: velocities and particle masses.
2.3	**MATERIALS RELATIONS**	**Relation**	Intramolecular forces for bonded and non-bonded interactions.
		Physical quantities/ descriptors for each MR	Intramolecular Parameters (bond and angle parameters (length, spring constant Torsional Parameters), are assumed to be fixed for the chemical structures of the matrix and the fillers. Non bonded parameters in the SCFT formulation are calculated with the help of □ parameters and density field compressibilities. The [taken from Polymer Handbooks. A mapping from non-bonded Lennard-Jones parameters and [used in this type of models. Compressibilities are taken from databases.
2.4	**PHYSICS FORMULATION OF THE CONDITIONS**		
2.5	**SIMULATED INPUT**		

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS	
3.1	NUMERICAL SOLVER	Velocity Verlet Algorithm for particle positions and velocities. For the Density Field and its derivative linear Interpolation on a lattice (Particle Mesh fashion for the non-bonded part)
3.2	SOFTWARE TOOL	OCCAM Software Developed at UNISA Software description and its parallelization strategy and benchmarks are reported in the Software News and Updates section of Journal of Computational Chemistry: Hybrid Particle-Field Molecular Dynamics Simulations: Parallelization and Benchmarks Ying Zhao, Antonio De Nicola, Toshihiro Kawakatsu, and Giuseppe Milano Journal of Computational Chemistry 33, 868, (2012) Software webpage http://www.smms.unisa.it/smms/occam
3.3	TIME STEP	0.13ps
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	Periodic boundary conditions in x, y and z directions are applied to mimic a homogeneous situation. In the present case, having Carbon Fibers (CF), also the macroscopic element (i.e. CF) will be conductive and then a generator of heat. In this case, the advantage of the grid representation chosen to modify the thermostat is related to the possibility of extending the boundaries beyond molecular scale models according to the geometry of CF set up.
3.6	ADDITIONAL SOLVER PARAMETERS	Specific parameters of Hybrid Particle Field Molecular Dynamics Simulations are the Density Field spatial and time resolution in the calculation obtained on the fly from particle positions. Mesh size and frequency of field update.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	Particle trajectories the coordinate of the fillers CNTs will be processed - to extract the network for model 2 - to have information about local conductivities (conductivity field □(r)) this quantity is be used in model 2 to determine the heat flux as post processing operation of Model 2. - Percolation threshol
4.2	METHODOLOGIES	Sigma is calculated as average of the conductivities in one cell. Percolation threshold is calculated fitting a power law from simulations at different concentrations
4.3	MARGIN OF ERROR	Not available.

Simulation with MODEL 2– Resistance Model

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Electrical transport and generated heat through a matrix material and heat generation
1.2	MATERIAL	Network calculated from post processing of model 1:  the chemical composition is taken into account when assigning intrinsic conductivities to different species. In the case of CNTs assembled in Polymer and Resin composites only the CNTs will be assumed to contribute to conductivity mechanism.
1.3	GEOMETRY	Size and form of the system is determined by Model 1.
1.4	TIME LAPSE	Nanoseconds
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	External voltage
1.6	PUBLICATION ON THIS DATA	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Electricity (Kirchhoff)Model applied to Percolation (Resistor Network Approach)	
2.1	MODEL ENTITY	3D network of resistances.	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Kirchhoff (Maxwell eq) and electrical Heat flow generation The potential difference and the resistance between connected grid points is used to calculate the current between the two points using Ohms law: $V=RI$

		Physical quantities	Resistances and their position in the simulation box and the generated heat flux as post-processing
2.3	**MATERIALS RELATIONS**	**Relation**	Configurational calculation of resistances. As explained below values of resistance are calculated on the basis of the position of CNT's particles in the simulation box. Internal resistance of a CNT $$R_{ij} = \frac{4l_{jk}}{\pi\sigma_{CNT}D^2}$$ Contact resistance between CNT pairs Landauer–Buttiker formula: $$R_{contact} = \frac{h}{2e^2}\frac{1}{MP}$$
		Physical quantities/ descriptors for each MR	l_{jk} =CNT length σ_{CNT} and D are the intrinsic conductivity and the diameter of the CNT, respectively. Each pair of CNT produces a contact resistance if the distance between them was less than d_{cutoff}. h is Planck's constant, e is the electron charge $\frac{h}{2e^2}$ is the quantized resistance. M is the total number of conduction channels. Transfer probability P is given by $$P = \begin{cases} \exp\left(-\frac{d_{VdW}}{d_{tunnel}}\right) & \text{if} d \le D + d_{vdW} \\ \exp\left(-\frac{d}{d_{tunnel}}\right) & \text{if} D + d_{vdW} < d \le D + d_{cutoff} \end{cases}$$ Here $d_{tunnel} = \frac{h}{2\pi\sqrt{8m_e\Delta E}}$ is the lenghtscale for electron tunneling, me is the electron mass, barrier and d_{vdw}=0.34 nm is the van der Waals separation distance.
2.4	**PHYSICS FORMULATION OF THE CONDITIONS**	The conditions such as pressure, concentration of CNTs are fixed in the previous Model 1 (Coarse-Grained Molecular Dynamics) and affecting the CNT's distribution, relative distances and shape of CNT assemblies give rise to different network of resistances. The temperature changes from initial value set in model 1 according to the calculated heat flux as post-processing operation of Model 2 and Model 3.	
2.5	**SIMULATED INPUT**	The network is calculated from coordinates of CNTs of model 1 and conductivity from model 1 plus external heating condition obtained from post processing of Model 3.	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Resolution of a system of linear equation, matrix inversion and matrix multiplication. The size of the problem according to the description given in 2.2 Model Physics is smaller than the initial NxN (where N is the initial number of resistance). Research of percolation paths in the resistor network and elimination of internal nodes makes this calculation more efficient. This feature is very important in this case, where this calculation is made on the fly (see post processing).	
3.2	SOFTWARE TOOL	OCCAM Software Developed at UNISA Software description and its parallelization strategy and benchmarks are reported in the Software News and Updates section of Journal of Computational Chemistry: Software webpage http://www.smms.unisa.it/smms/occam	
3.3	TIME STEP	microsecond	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	Resistor network, resistance values and Cartesian positions x, y, z
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	Periodic Boundary conditions corresponding to particles configuration in model 1. For systems representing regions where the nanocomposite is in contact with carbon fibers determined by the geometry of Model 3.	
3.6	ADDITIONAL SOLVER PARAMETERS	No additional parameters are envisaged	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	The heat as fixed temperatures per volume will be given to Model 1 and for Model 3 the microscopic averaged conductivity is calculated.
4.2	METHODOLOGIES	Heat resulting from the current flow calculated using the power equation: $P=VI=Q$ In the present case, having carbon fibers as conductive element, additional heat can be included for the regions of the system eventually in contact with the carbon fiber. Microscopic averaged conductivity Conductivity will be averaged over several configurations (?) and provided as input for Model 3.
4.3	MARGIN OF ERROR	To be determined

Simulation with MODEL 3– Thermo-Electrical model at RUC scale

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Calculation of the heat generation due to an electrical current on a representative cell at microscale. Here we need to take into account the third materials components which are microscale fibers
1.2	MATERIAL	Material are - carbon-based nanofillers embedded into a polymer matrix. Electrical properties will be given by model 2. - Carbon Fibers Electrical properties given by model 2 The other properties will be obtained either from Material supplier, either from public literature, either from characterization carried out in WP5 of the MASTRO project.
1.3	GEOMETRY	The geometry will correspond to a cubic periodic box that represents the composite statistically. The RUC will contain the conductive network calculated from model 2 and the polymer. Dimension should be in the range of few micrometers.
1.4	TIME DURATION OF THE TOTAL PROCESS	Regarding self-heating application, the order of magnitude will be a second.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	A low voltage and imposed current The ambient temperature
1.6	PUBLICATION ON THIS DATA	-

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Tightly coupled Continuum models : Heat flow coupled with electrics	
2.1	MODEL ENTITY	Finite elements	
2.2	MODELPHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Steady-state conservation of charge equation $$\nabla J = 0$$ $$E = -\nabla V$$ Energy equation written for Temperature $$\rho Cp(T)\frac{\partial T}{\partial t} = \nabla.(-\lambda(T)\nabla T) + Q$$ Equation 1 and 2 are coupled through the joule heating

			relation
		Physical quantities	Equations are solved for each phase, which means physical quantities appears both for homogenised polymer/CNT and glass fiber □ density Cp : Specific heat l : Thermal conductivity Q : Heat flux J : electrical current density E: Electric field intensity V : Electric scalar potential
2.3	**MATERIALS RELATIONS**	**Relation**	Joule heating $Q = \sigma(T)(-\nabla V)^2$ $Q = J.E$
		Physical quantities/ descriptors for each MR	□ : Electrical conductivity Q : Heat flux V: Electrical potential J : electrical current density E: Electric field intensity
2.4	**PHYSICS FORMULATION OF THE CONDITIONS**	Thermal boundary conditions : $T(t = 0) = T_{initial}$ defined by the user On boundaries : $-\lambda_1(T_1)\frac{\partial T_1}{\partial n}\Big\|_{\Gamma_2} = 0$ Electrical boundary conditions : $V = V_0$ is the imposed electrical potential $J.\vec{n} = J_0.\vec{n}$ is the imposed current density	
2.5	**SIMULATED INPUT**	Effective electrical conductivity calculated by model 2	

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**	
3.1	**NUMERICAL SOLVER**	Mesh parameters • Mesh 3D • Mesh with shellelement We use to solve this problem an implicit approach. Finite Element Method

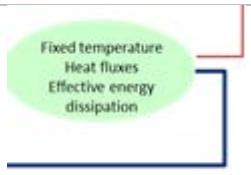
3.2	**SOFTWARE TOOL**	Abaqus from SIMULIA Platform, Comsol Multiphysiscs or FreeFEM	
3.3	**TIME STEP**	The timestep would correspond to few microseconds.	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	The following FE equations couple electromagnetism equations to energy equation. $$\begin{bmatrix}[Ct] & [0]\\ [0] & [Cv]\end{bmatrix}\begin{Bmatrix}\dot{T}\\ \dot{V}\end{Bmatrix}+\begin{bmatrix}[Kt] & [0]\\ [0] & [Kv]\end{bmatrix}\begin{Bmatrix}T\\ V\end{Bmatrix}=\begin{Bmatrix}Q\\ I\end{Bmatrix}$$ [Ct] :thermal specific heat matrix [Cv] :dielectric coefficient matrix [Kt] : thermal conductivity matrix [Ct] :electrical conductivity matrix {T} :temperature {V} : electric potential {Q} : heat generation rate per unit volume {I} : applied nodal electric current vector
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**		
3.6	**ADDITIONAL SOLVER PARAMETERS**		

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT**	Main output are : T : Temperature q :heat flux J : electrical current density E: Electric field intensity V : Electric scalar potential The effective electrical conductivity can be computed by averaging over all control volumes.
4.2	**METHODOLOGIES**	We need to postprocess the evolution of the heat dissipation as a function of the electrical current density or the electrical field intensity thanks to the Joule heating relation. Heat produced by the carbon fibers will be added as additional heat (Q) to the condition of Model 1. (As we have three components at different scale (polymer, nanofillers, microfillers), we need to perform a double homogenization) Finally a homogenisation is applied to obtain the effective heat generation on the RUC.
4.3	**MARGIN OF ERROR**	We cannot estimate this point yet

Simulation with MODEL 4– Thermo-Electrical model at macroscale

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Calculation of the heat generation due to an electrical current on a part.
1.2	MATERIAL	Material are - carbon-based nanofillers embedded into a polymer matrix. Electrical properties will be given by model 2. - Glass fibers The other properties will be obtained either from public literature, either from characterization carried out in WP5 of the MASTRO project.
1.3	GEOMETRY	The geometry will correspond to an industrial part. Dimension in the range of few millimeters or few meters.
1.4	TIME LAPSE	Regarding selfheating application, the order of magnitude will be the second.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	A low voltage and imposed current The ambient temperature
1.6	PUBLICATION ON THIS DATA	-

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum model : Heat flow coupled with electrics	
2.1	MODEL ENTITY	Finite elements	
2.2	MODELPHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Energy equation written for Temperature $$\rho Cp(T)\frac{\partial T}{\partial t} = \nabla.(-\lambda(T)\nabla T) + Q$$ Steady-state conservation of charge equation $$\nabla J = 0$$ $$E = -\nabla V$$ Equation 1 and 2 are coupled through the joule heating relation

		Physical quantities	Equation are solved for each phase, that mean physical quantities appears both for polymer and glass fibers. ρ : density Cp : Specific heat l : Thermal conductivity Q : Heat flux J : electrical current density E: Electric field intensity V : Electric scalar potential The temperature T and the potential are the unknown parameters. As the problem is time-dependant and solved in 3D, the output are matrices T(x,y,z,t) and V(x,y,z,t)
2.3	**MATERIALS RELATIONS**	**Relation**	Joule heating $\mathrm{Q} = \mathrm{K}_{v\,\mathrm{eff}}(\mathrm{T})(-\nabla \mathrm{V})^2$ $\mathrm{Q} = \mathrm{J}.\mathrm{E}$
		Physical quantities/ descriptors for each MR	$\mathrm{K}_{v\,\mathrm{eff}}$: effective electrical conductivity Q : Heat flux V: Electrical potential J : electrical current density E: Electric field intensity
2.4	**PHYSICS FORMULATION OF THE CONDITIONS**	Thermal boundary conditions : $T(t=0) = T_{initial}$ defined by the user On boudaries : $-\lambda_1(T_1)\left.\frac{\partial T_1}{\partial n}\right\|_{\Gamma_2} = 0$ Electrical boundary conditions: $\mathrm{V} = \mathrm{V}_0$ is the imposed electrical potential $\mathrm{J}.\vec{\mathrm{n}} = \mathrm{J}_0.\vec{\mathrm{n}}$ is the imposed current density	
2.5	**SIMULATED INPUT**	 from model 3	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Finite Element Method	
3.2	SOFTWARE TOOL	Abaqus from SIMULIA Platform, Comsol Multiphysics or FreeFEM	
3.3	TIME STEP	The timestep would correspond to few microseconds.	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	The following FE equations couple electromagnetism equations to energy equation. $$\begin{bmatrix}[Ct] & [0]\\ [0] & [Cv]\end{bmatrix}\begin{Bmatrix}\dot{T}\\ \dot{V}\end{Bmatrix}+\begin{bmatrix}[Kt] & [0]\\ [0] & [Kv]\end{bmatrix}\begin{Bmatrix}T\\ V\end{Bmatrix}=\begin{Bmatrix}Q\\ I\end{Bmatrix}$$ [Ct] :thermal specific heat matrix [Cv] :dielectric coefficient matrix [Kt] : thermal conductivity matrix [Ct] :electrical conductivity matrix {T} : temperature {V} : electric potential {Q} : heat generation rate per unit volume {I} : applied nodal electric current vector
3.5	COMPUTATIONAL BOUNDARY CONDITIONS		
3.6	ADDITIONAL SOLVER PARAMETERS		

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	Main output are : T : Temperature q : heat flux J : electrical current density E: Electric field intensity V : Electric scalar potential
4.2	METHODOLOGIES	We calculate in a first time the electrical current density and at the same time the effective heat generation in the part. The heat generation will give us the temperature field in the part.
4.3	MARGIN OF ERROR	We cannot estimate this point yet