

## Deliverable D1.2

### Description of the modeling workflow according with CWA17284

Deliverable information	
<b>Responsible Partner::</b>	VTT
<b>Work Package</b>	WP1
<b>Contributing Partner(s):</b>	VTT, ACS, UMR, UNIBO
<b>Dissemination Level<sup>1</sup>:</b>	PU
<b>Type:</b>	R
<b>Due Date:</b>	30.6.2023
<b>Submission Date:</b>	30.6.2023
<b>Version:</b>	1.1

<sup>1</sup> PU = PUBLIC fully open ((warning) automatically posted online on the Project Results platforms)

SEN = Sensitive – limited under the conditions of the Grant Agreement

EUCI = EU classified under Decision 2015/444





## Project Profile

<b>Programme</b>	HORIZON EUROPE
<b>Call</b>	HORIZON-CL4-2022-RESILIENCE-01
<b>Topic</b>	HORIZON-CL4-2022-RESILIENCE-01-19 - Advanced materials modelling and characterisation (RIA)
<b>Number</b>	101092211
<b>Acronym</b>	CoBRAIN
<b>Title</b>	Integrated Computational-Experimental Material Engineering of Thermal Spray Coatings (CoBRAIN)
<b>Start Date</b>	1 January 2023
<b>Duration</b>	48 months

## Document History

Version	Date	Entity	Remarks
<b>0.0</b>	20.5.2023	VTT, ACS	1 <sup>st</sup> draft
<b>1.0</b>	26.6.2023	ACS	Additions for platforms
<b>1.1</b>	30.6.2023	VTT, UMR	Submission version



## Publishable Summary<sup>2</sup>

The report summarises the description of the interoperable material modelling workflow according to CWA17284 for the CoBRAIN project. It mainly consists of 3 sub-workflows the key elements of which a

1. **Alloy design (MATERIAL):** CALPHAD and phase field (PF) modelling and screening of elemental compositions, supplemented by density-functional theory (DFT) based calculations of more complex and multi-component systems. DFT also to support parameterization of solidification and mechanical property models.
2. **Process and coating solidification modelling (PROCESS):** Computational fluid dynamics (CFD) and particle based flow modeling of the coating deposition process; phase-field (PF) modelling of “splat” microstructure evolution.
3. **Properties modelling (PROPERTY):** Crystal plasticity and modelling of, e.g., mechanical properties (for example, stress-strain response) of solidified microstructures.

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<sup>2</sup> This summary will be used for public dissemination of CoBRAIN’s activities



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## Abbreviations

Abbreviation	Definition
CALPHAD	CALculation of PHase Diagrams
CP	Crystal Plasticity
DFT	Density Functional Theory
TCHEA	High Entropy Alloys Database by Thermocalc
ML	Machine Learning
HEA	High-Entropy Alloy
HEC	High-Entropy Carbide
RVE	Representative Volume Element
VOF	Volume-of-Fluid
FE	Finite Element
PF	Phase-Field



# 1 Alloy design (MATERIAL)

## 1.1 MODA for computational HEA composition screening applying thermodynamic, phase field and density functional theory models

Simulated in the CoBRAIN project

Data owner [Access, [info@access-technology.de](mailto:info@access-technology.de)]

Table 1.1. Overview of the simulations

Overview of the simulation		
1	<b>User case</b>	Computational screening of high entropy alloys by computing phase fractions, alloy element distribution and microstructure for a thermodynamic equilibrium and under process conditions during particle flight from the nozzle until impact.
2	<b>Chain of models (used in the simulation)</b>	Model 1   Continuum thermodynamics (CALPHAD).
		Model 2   Multiphase/Multicomponent phase field model linked to CALPHAD database (continuum).
		Model 3   Density functional theory and ab initio molecular dynamics (DFT)
3	<b>Publication peer-reviewing the data</b>	Not yet available.
4	<b>Access conditions</b>	Phase-field software MICRESS owned by Access e.V., <a href="http://www.micress.de">www.micress.de</a> (commercial, licence required), Thermodynamic software Thermocalc and TCHEA databases owned by Thermo-Calc AB, <a href="http://www.thermocalc.se">www.thermocalc.se</a> (commercial, licence required). The DFT software VASP owned by VASP Software GmbH, <a href="http://www.vasp.at">www.vasp.at</a> (commercial license may be required).
5	<b>Workflow and its rationale</b>	CALPHAD is the state-of-the-art approach for a comprehensive thermodynamic material description. Phase-field models are the state-of-the-art models for simulating the evolution of complex microstructures. They combine the governing physical mechanisms, thermodynamic driving forces, transport by diffusion and kinetic and curvature effects of an interface. DFT modeling can be utilized to investigate and calculate various material properties and metrics ab initio.



Table 1.2. Workflow

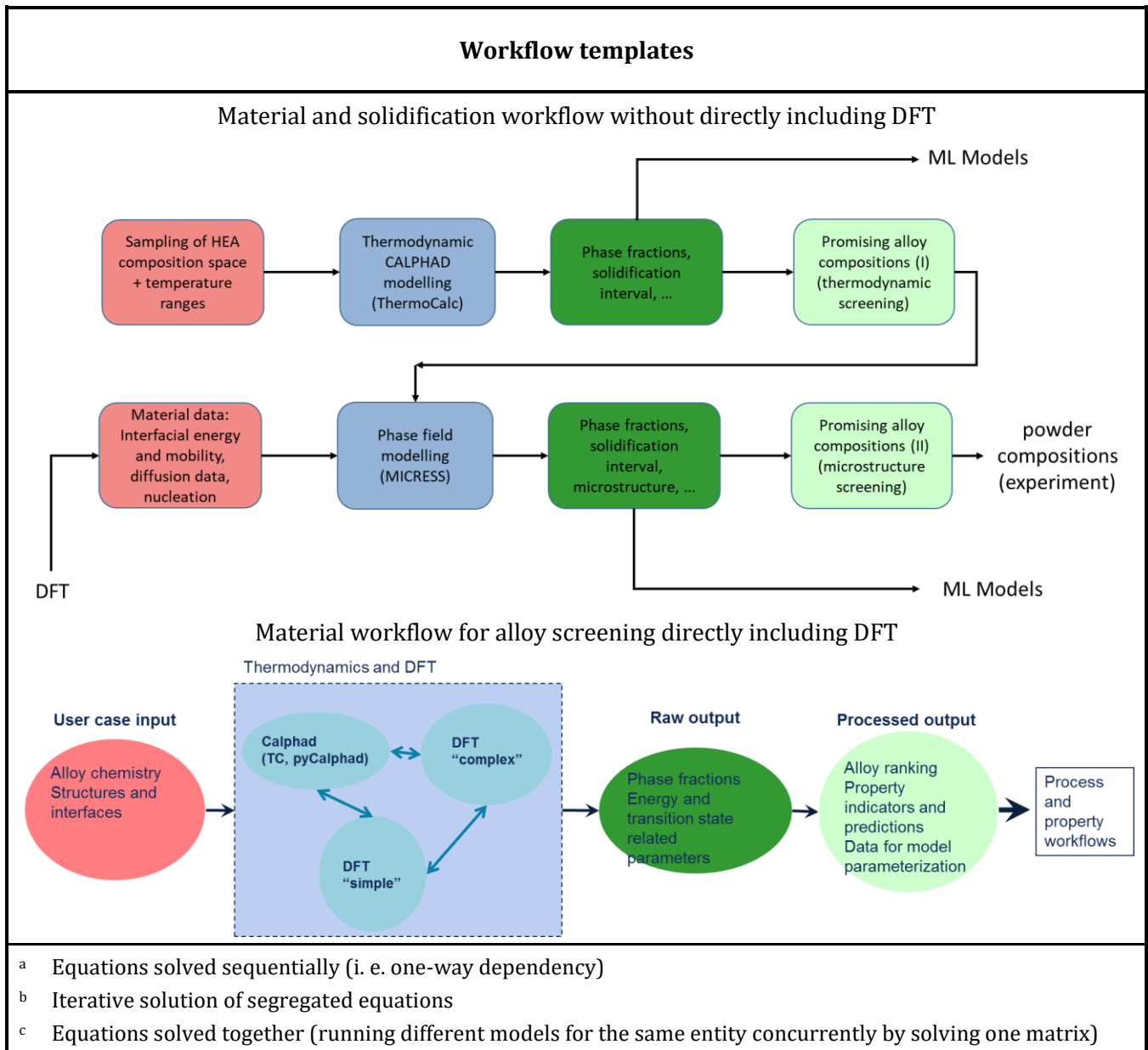




Table 1.3 Aspect of the user case / system to be simulated, model 1

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 1</b>	Computational screening to identify promising alloy compositions based on thermodynamic equilibrium properties, in particular phase fractions, solidification interval and thermal contraction.
1.2	<b>Material</b>	High Entropy Alloys (HEA) with 5-6 principal elements with or without hard metallic inclusions.
1.3	<b>Geometry</b>	No geometry, 1 mol of atoms.
1.4	<b>Time lapse</b>	No time laps, equilibrium state (invariant).
1.5	<b>Manufacturing process or in-service conditions</b>	Predefined conditions for the state variables p, T and $c_i$ . T ranges from room temperature to evaporation temperature, p ranges from 100 mbar to 1 bar, the alloy composition $c_i$ (concentration of alloying element i) is varied to probe the whole composition range. Alloying elements are Al, Ni, Fe, Co, Cr, Mn.
1.6	<b>Publication on this data</b>	Not yet available.



Table 1.4. Governing equations, model 1

2		Governing equations	
2.1	<b>Model type and name</b>	Computational thermodynamics (CALPHAD)	
2.2	<b>Model entity</b>	The entity in this physics-based model is continuum volume.	
2.3	<b>Physics equation</b>	Equation	$G(p, T, c^i) = \sum_{\alpha} f_{\alpha} G_{\alpha} \rightarrow \min$ (minimisation of the free energy of a system)
		Physics quantities	G: Gibbs free energy of a phase $\alpha$ . $f_{\alpha}$ : phase fraction of phase $\alpha$ . p: system pressure, T temperature.
2.4	<b>Materials relations</b>	Relation	Equilibrium relation between thermodynamic state variables.
		Physics quantities for each materials relation	Composition (element concentration) of a certain phase. The Gibbs energy density of a certain phase is defined by polynomial functions, its coefficients are derived from a data assessment following the CALPHAD approach.
2.5	<b>Simulated input</b>		

Table 1.5. Solver and computational translation of the specification, model 1

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	Newton-Raphson and solvers for sets of linear equations.	
3.2	<b>Software tool</b>	Thermo-Calc ( <a href="http://www.thermocalc.se">www.thermocalc.se</a> )	
3.3	<b>Time step</b>	Not applicable.	
3.4	<b>Computational representation</b>	Physics equation	
		Material relations	Polynomial descriptions of the Gibbs-energy stored in the CALPHAD database.
		Material	The parameters for the Gibbs-energy functions are stored in the database, in case of the commercial databases TCHEA, values are crypted.
3.5	<b>Computational boundary conditions</b>	Not applicable.	
3.6	<b>Additional solver parameters</b>	Numerical parameter to control the numerical efficiency of the solver may be adjusted depending on particular conditions.	



Table 1.6. Post-processing, model 1

4		Post-processing
4.1	<b>The processed output</b>	Raw output are thermodynamic state variables. From the state variables, material properties can be determined using appropriate property models. Criteria functions (to be developed) will be used to identify promising alloy compositions.
4.2	<b>Methodologies</b>	To be developed in the project.
4.3	<b>Margin of error</b>	Not applicable.

Table 1.7. Aspect of the user case / system to be simulated for model 2

1		Aspect of the user case / system to be simulated
1.1	<b>Aspect of the user case to be simulated using model 2</b>	Based on a pre-defined alloy composition and a predefined representative volume (RVE), the microstructure evolution is simulated beginning with a (partially) molten particle, ending up at the state before impact. Thermal process condition and parameters of a nucleation model is user input.
1.2	<b>Material</b>	High entropy alloys (HEA's) with 5-6 principal elements with or without hard metallic inclusions.
1.3	<b>Geometry</b>	A single, almost spherical powder particle in the size range of diameter $d=20\ \mu\text{m}$ to $50\ \mu\text{m}$ .
1.4	<b>Time lapse</b>	Time during flight from nozzle to target, typically $t = 100\ \text{ms}$ to $1\ \text{s}$ .
1.5	<b>Manufacturing process or in-service conditions</b>	Heat transfer from the particle to its environment (heat loss caused by radiation and heat transfer into the gas environment)
1.6	<b>Publication on this data</b>	Not yet available.



Table 1.8. Governing equations for model 2

2		Governing equations	
2.1	<b>Model type and name</b>	Multiphase field model.	
2.2	<b>Model entity</b>	The entity in this physics-based model is continuum volume.	
2.3	<b>Physics equation</b>	Equation	<p>Phase field equation:</p> $\dot{\phi}_\alpha = \frac{1}{n} \sum_\beta \mu_{\alpha\beta} \left( \frac{\delta f}{\delta \phi_\alpha} - \frac{\delta f}{\delta \phi_\beta} \right) = \frac{1}{n} \sum_\beta \mu_{\alpha\beta} \left( I_{\alpha\beta} + \Delta G_{\alpha\beta}^{\text{chem}} \right)$ <p>Multicomponent diffusion equation:</p> $\dot{c}^i = \sum_\alpha \nabla M_\alpha^i \phi_\alpha \nabla \frac{\delta f}{\delta c_\alpha} = \sum_\alpha \nabla M_\alpha^i \phi_\alpha \left( \frac{\delta^2 f}{\delta c_\alpha^2} \nabla c_\alpha^i \right)$ <p>Heat conservation (temperature)</p> $\int_V \sum_\alpha \rho_\alpha c_\alpha^p \dot{T} = \int_V \sum_\alpha H_\alpha(T, c_i) \dot{\phi}_\alpha + \dot{Q}$
		Physics quantities	A set of phase field order parameters $\phi_\alpha$ , one for each grain $\alpha$ . $c^i(x,y,z)$ , concentration fields, one for each alloying element $i$ . Temperature field $T(x,y,z)$ .
2.4	<b>Materials relations</b>	Relation	<p>Proportionality <math>\mu_{\alpha\beta}</math> between interface velocity and driving forces, <math>I_{\alpha\beta}</math> is the interface contribution, <math>\Delta G</math> the thermodynamic contribution.</p> <p><math>M^i</math>, the atomistic mobility connecting gradients in the chemical potential with diffusion fluxes.</p> <p>Thermodynamic relations between the different state variables.</p>
		Physics quantities for each materials relation	<p>Interfacial mobility <math>\mu = \mu(\alpha, \beta, \gamma, T)</math>, <math>\alpha, \beta, \gamma</math> are Euler angles determining the crystal orientation.</p> <p>From the atomistic mobilities <math>M^i</math> the diffusion matrix <math>D^{ij}</math> is calculated to solve Fick's equation.</p> <p>Enthalpies <math>H_\alpha</math> and heat capacity <math>c_\alpha^p</math> for each phase <math>\alpha</math>, both as function of <math>T</math> and <math>c^i</math>.</p>
2.5	<b>Simulated input</b>		



Table 1.9. Solver and computational translation of the specification for model 2

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	Finite differences.	
3.2	<b>Software tool</b>	MICRESS	
3.3	<b>Time step</b>	Adaptive from numerical stability criteria.	
3.4	<b>Computational representation</b>	Physics equation	For diffusion: Fick's equation: $\dot{\bar{c}}(\mathbf{x}, t) = \nabla \sum_{\alpha} \phi_{\alpha} \bar{\bar{D}}_{\alpha} \nabla \bar{c}_{\alpha}$
		Material relations	Thermodynamic driving forces are derived from local equilibrium calculations. Interfacial contributions to the driving force are derived from the local interface curvature.  Interface mobility for the phase field equation is given in temperature-dependent form in an ascii-table. Anisotropies are defined as a series of spherical harmonics. Coefficients are user-input. Diffusion coefficients are defined by Arrhenius expressions (activation energy and pre-factor)
		Material	Gibbs-free energy expressed by a series of polynomial descriptions in the CALPHAD database for thermodynamic quantities.  Interfacial energy is a user input and defined as temperature dependent values provided by an ascii table.
3.5	<b>Computational boundary conditions</b>	Adiabatic conditions superimposed by an external heat flux (energy balance).  Periodic or adiabatic for phase-field and concentration fields depending on the simulation scenario.	
3.6	<b>Additional solver parameters</b>	Cut-off value for minimal fraction of the phase field order parameter.	



Table 1.10. Post-processing for model 2

4		Post-processing
4.1	<b>The processed output</b>	Average phase fraction, element distribution and solidification interval are primary outputs. Based on evaluation criteria, the processed output should be alloy compositions which fulfil certain user defined criteria.
4.2	<b>Methodologies</b>	Volume averaging.
4.3	<b>Margin of error</b>	Numerical errors are caused by different grid resolutions. A grid independent resolution with <5% changes upon further refinement can be achieved for typical conditions and affordable computational costs. This margin relates to numerical errors for a particular set of material parameters. Major uncertainties in comparison to physical experiments are determined by uncertainties in the material parameters. Another source of uncertainties is the stochastic nature of microstructure evolution. This could be tackled by larger domains or averaging over many individual simulations.



Table 1.11. Aspect of the user case / system to be simulated for model 3

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 3</b>	Computational screening to identify promising alloy compositions based on ab initio calculated properties and metrics. Calculations carried out with simpler and cheaper high-throughput metrics ("SIMPLE" in the MODA) and costlier models of greater complexity ("COMPLEX" in the MODA).
1.2	<b>Material</b>	High Entropy Alloys (HEA) and High Entropy Carbides (HEC) with 5-6 principal elements or less.
1.3	<b>Geometry</b>	Lattice, supercell
1.4	<b>Time lapse</b>	Equilibrium state calculations
1.5	<b>Manufacturing process or in-service conditions</b>	Predefined conditions associated with pressure (p) and temperature (T) in cases and for computational metrics where can be necessary. The cases typically link, e.g., materials chemistry to specific materials properties, and as such do not contain information on process or in-service conditions.
1.6	<b>Publication on this data</b>	Not yet available.



Table 1.12. Governing equations, model 3

2		Governing equations	
2.1	<b>Model type and name</b>	Density functional theory (DFT)	
2.2	<b>Model entity</b>	The entity in this physics-based model is electron.	
2.3	<b>Physics equation</b>	Equation	Electronic Schrödinger equation: $\hat{H}\Psi = [\hat{T} + \hat{V} + \hat{U}]\Psi = \left[ \sum_{i=1}^N \left( -\frac{\hbar^2}{2m_i} \nabla_i^2 \right) + \sum_{i=1}^N V(\mathbf{r}_i) + \sum_{i<j}^N U(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi = E\Psi,$
		Physics quantities	$\hat{H}$ is the Hamiltonian, E is the total energy, T is the kinetic energy, V is the potential energy from the external field due to positively charged nuclei, and $\hat{U}$ is the electron–electron interaction energy.
2.4	<b>Materials relations</b>	Relation	Wavefunction satisfying the many-electron Schrödinger equation.
		Physics quantities for each materials relation	Elemental chemistry of a certain structure and phase.
2.5	<b>Simulated input</b>		



Table 1.13. Solver and computational translation of the specification for model 3

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	ab initio quantum mechanical solver	
3.2	<b>Software tool</b>	VASP ( <a href="http://www.vasp.at">www.vasp.at</a> )	
3.3	<b>Time step</b>	Not applicable.	
3.4	<b>Computational representation</b>	Physics equation	See 2.3.
		Material relations	Projector augmented wave, plane wave basis set, pseudopotentials
		Material	Functionals, potentials
3.5	<b>Computational boundary conditions</b>	Unit cell with periodic boundary conditions, surfaces, interfaces.	
3.6	<b>Additional solver parameters</b>	Solver parameters are incorporated and adjusted depending on particular analysis needs.	



Table 1.14. Post-processing for model 3

4		Post-processing
4.1	<b>The processed output</b>	Various energy related metrics, transition state parameters, calculated properties: Cauchy pressure, elasticity, formation energies, Rice criterion (stacking fault energies, surface/cohesion/formation energies), energies for short range ordering, lattice constants/misfits, phase & lattice specific formation/cohesive/interface/defect energies, free energies (phonon calculations), phase stabilities, solubility.
4.2	<b>Methodologies</b>	Specific post-processing methodologies to be implemented during the project as part of the computational workflows.
4.3	<b>Margin of error</b>	Maximum 5% deviation from any experimental references.



## 2 Process and coating solidification modelling (PROCESS)

### 2.1 MODA for thermal spray process modeling

Simulated in project CoBRAIN

Data owner [VTT Technical Research Centre of Finland Ltd., [Anssi.Laukkanen@vtt.fi](mailto:Anssi.Laukkanen@vtt.fi)]

Table 2.1. Overview of the simulations

Overview of the simulation			
1	<b>User case</b>	Coupled simulation making use of continuum and discrete flow modeling and phase field modeling of solidification is utilized to simulate the thermal spray coating deposition processes.	
2	<b>Chain of models (used in the simulation)</b>	Model 1	Fluid mechanics model (continuum, discrete)
		Model 2	Phase field model (continuum)
3	<b>Publication peer-reviewing the data</b>	Not yet available.	
4	<b>Access conditions</b>	Fluid mechanics modeling makes use of the OpenFOAM solver ( <a href="https://www.openfoam.com/">https://www.openfoam.com/</a> ) available as open source, phase field model "OpenPF" is internally developed by VTT.	
5	<b>Workflow and its rationale</b>	Computational fluid mechanics (CFD) is used to address particle behavior in-flight during the thermal spray deposition process, either utilizing methods such as multiphase volume-of-fluid (VOF) without or with discrete modeling entities. Following coating deposition, phase field modeling is used to simulate the solidification process. This simulation can include, as seen necessary, further convective or thermomechanical coupling effects.	



Table 2.2. Workflow

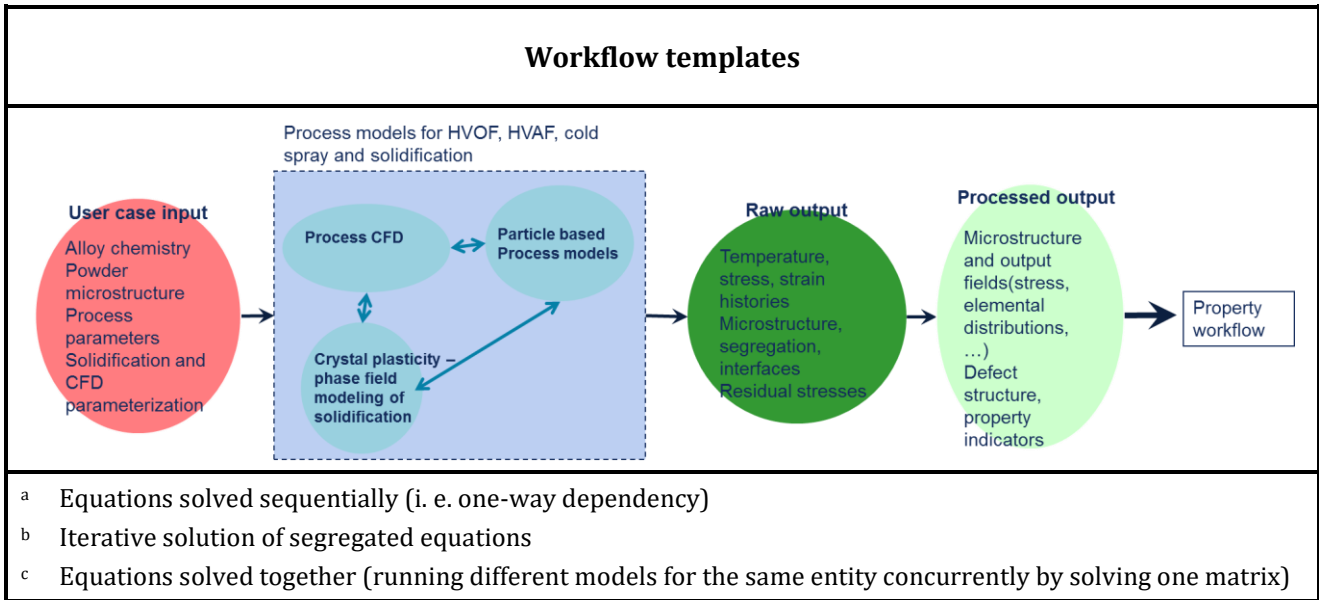




Table 2.3. Aspect of the user case / system to be simulated, model 1

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 1</b>	Thermal spray deposition is used for the HEA/HEC coatings, the modeling and simulation of the coating deposition process is used to identify most suited process parameters for specific powder-process combinations.
1.2	<b>Material</b>	High Entropy Alloys (HEA) with 5-6 principal elements with or without hard metallic inclusions.
1.3	<b>Geometry</b>	The geometry of the system will be equivalent to the representative experimental manufacturing process setup.
1.4	<b>Time lapse</b>	Time lapse is equivalent to the experimental manufacturing processes for coating deposition.
1.5	<b>Manufacturing process or in-service conditions</b>	Process parameters (such as temperature, initial velocities, mass flow) will be extracted directly from coating manufacturing trials and experiments.
1.6	<b>Publication on this data</b>	Not yet available.



Table 2.4. Governing equations, model 1

2		Governing equations	
2.1	<b>Model type and name</b>	Computational fluid dynamics (CFD)	
2.2	<b>Model entity</b>	The entity in this physics-based model is continuum volume.	
2.3	<b>Physics equation</b>	Equation	Navier-Stokes equations in convective form: $\rho \frac{D\mathbf{u}}{Dt} = \rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \cdot \left\{ \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \zeta (\nabla \cdot \mathbf{u}) \mathbf{I} \right\} + \rho \mathbf{g}.$
		Physics quantities	$\frac{D}{Dt}$ is the material derivative, $\rho$ the mass density, $\mathbf{u}$ the flow velocity, $p$ is the pressure, $t$ is the time, $\boldsymbol{\tau}$ the deviatoric stress tensor and $\mathbf{g}$ volumetric accelerations.
2.4	<b>Materials relations</b>	Relation	In general, we consider compressible flow
		Physics quantities for each materials relation	Bulk and dynamic viscosity, density, Lamé parameters
2.5	<b>Simulated input</b>	Powder characteristics (size, shape distributions) and microstructure obtained from characterisation or simulation.	



Table 2.5. Solver and computational translation of the specification, model 1

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	Finite volume method, finite element, discrete	
3.2	<b>Software tool</b>	OpenFOAM (openfoam.com)	
3.3	<b>Time step</b>	Depending on the convergence study aiming to obtain the most accurate results with the largest possible time step.	
3.4	<b>Computational representation</b>	Physics equation	As provided in 2.3
		Material relations	As provided in 2.4
		Material	Continuous multi-phase distribution of material
3.5	<b>Computational boundary conditions</b>	Finite domain with boundary and initial conditions based on discretization of the experimental manufacturing processes.	
3.6	<b>Additional solver parameters</b>	Numerical parameters to control the numerical efficiency of the solver may be adjusted depending on particular conditions.	



Table 2.6. Post-processing, model 1

4	Post-processing	
4.1	<b>The processed output</b>	Deposited coating thermal and mechanical history, defects.
4.2	<b>Methodologies</b>	Post-processing scripts.
4.3	<b>Margin of error</b>	Maximum 5% deviation from experimental reference.



Table 2.7. Aspect of the user case / system to be simulated, model 2

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 2</b>	Solidification of the coating and formation of its respective microstructure and interfaces/interphases.
1.2	<b>Material</b>	High Entropy Alloys (HEA) with 5-6 principal elements with or without hard metallic inclusions.
1.3	<b>Geometry</b>	The geometry of the system will be equivalent to the representative experimental manufacturing process setup, particularly the coating and its microstructure.
1.4	<b>Time lapse</b>	Time lapse is equivalent to the experimental manufacturing processes for coating deposition.
1.5	<b>Manufacturing process or in-service conditions</b>	Process parameters (such as temperature, initial velocities, mass flow) will be provided directly by the preceding model 1 performing CFD based analysis of the coating deposition process.
1.6	<b>Publication on this data</b>	Not yet available.



Table 2.8. Governing equations, model 2

2		Governing equations	
2.1	<b>Model type and name</b>	Phase field modeling (PF)	
2.2	<b>Model entity</b>	The entity in this physics-based model is continuum volume.	
2.3	<b>Physics equation</b>	Equation	<p>Phase field equation:</p> $\dot{\phi}_\alpha = \frac{1}{n} \sum_\beta \mu_{\alpha\beta} \left( \frac{\delta f}{\delta \phi_\alpha} - \frac{\delta f}{\delta \phi_\beta} \right) = \frac{1}{n} \sum_\beta \mu_{\alpha\beta} (I_{\alpha\beta} + \Delta G_{\alpha\beta}^{chem})$ <p>Multicomponent diffusion equation:</p> $c^i = \sum_\alpha \nabla M^i \phi_\alpha \nabla \frac{\delta f}{\delta c_\alpha} = \sum_\alpha \nabla M^i \phi_\alpha \left( \frac{\delta^2 f}{\delta c_\alpha^2} \nabla c_\alpha^i \right)$ <p>Heat conservation (temperature)</p> $\int_V \sum_\alpha \rho_\alpha c_\alpha^p \dot{T} = \int_V \sum_\alpha H_\alpha(T, c_i) \dot{\phi}_\alpha + \dot{Q}$
		Physics quantities	A set of phase field order parameters $\phi_\alpha$ , $c^i(x,y,z)$ , concentration fields, one for each alloying element i. Temperature field $T(x,y,z)$ .
2.4	<b>Materials relations</b>	Relation	<p>Proportionality <math>\mu_{\alpha\beta}</math> between interface velocity and driving forces, <math>I_{\alpha\beta}</math> is the interface contribution, <math>\Delta G</math> the thermodynamic contribution.</p> <p><math>M^i</math>, the atomistic mobility connecting gradients in the chemical potential with diffusion fluxes.</p>
		Physics quantities for each materials relation	<p>Interfacial mobility <math>\mu = \mu(\alpha, \beta, \gamma, T)</math>, <math>\alpha, \beta, \gamma</math> are Euler angles determining the crystal orientation.</p> <p>From the atomistic mobilities <math>M^i</math> the diffusion matrix <math>D^{ij}</math> is calculated to solve Fick's equation.</p> <p>Enthalpies <math>H_\alpha</math> and heat capacity <math>c_p^\alpha</math> for each phase <math>\alpha</math>, both as function of <math>T</math> and <math>c^i</math>.</p>
2.5	<b>Simulated input</b>	Thermal solution, convection, elemental distribution, thermomechanics will be provided by Model 1.	



Table 2.9. Solver and computational translation of the specification, model 2

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	Finite elements.	
3.2	<b>Software tool</b>	OpenPF in-house solver by VTT.	
3.3	<b>Time step</b>	Adaptive time stepping based on numerical convergence criteria.	
3.4	<b>Computational representation</b>	Physics equation	As provided in 2.3
		Material relations	Thermodynamic driving forces are derived from local equilibrium calculations. Interfacial contributions to the driving force is derived from the local interface curvature. Interface mobility for the phase field equation is given in temperature-dependent form in an ascii-table. Anisotropies are defined as a series of spherical harmonics. Coefficients are user input. Diffusion coefficients are defined by Arrhenius expressions (activation energy and pre-factor)
		Material	Gibbs-free energy expressed in the CALPHAD database for thermodynamic quantities.
3.5	<b>Computational boundary conditions</b>	Periodic and free surface boundary conditions	
3.6	<b>Additional solver parameters</b>		



Table 2.10. Post-processing, model 2

4	Post-processing	
4.1	<b>The processed output</b>	Deposited coating microstructure.
4.2	<b>Methodologies</b>	Post-processing scripts.
4.3	<b>Margin of error</b>	Maximum 10% deviation from experimental reference.



### 3 Properties modelling (PROPERTY)

#### 3.1 MODA for property and micromechanical modeling

Simulated in the CoBRAIN project

Data owner [VTT Technical Research Centre of Finland Ltd., [Anssi.Laukkanen@vtt.fi](mailto:Anssi.Laukkanen@vtt.fi)]

Table 3.1. Overview of the simulations

Overview of the simulation			
1	<b>User case</b>	Multiscale material simulations for predicting properties of high entropy alloy produced by the thermal spray coatings.	
2	<b>Chain of models (used in the simulation)</b>	Model 1	Micromechanics/Solid mechanics (continuum)
		Model 2	Density functional theory (DFT) (electronic)
3	<b>Publication peer-reviewing the data</b>	Not yet available	
4	<b>Access conditions</b>	Micromechanics and corrosion software is based on Finite Element software Z-set ( <a href="http://www.zset-software.com/">http://www.zset-software.com/</a> ) owned by ARMINES & ONERA THE FRENCH AEROSPACE LAB, ABAQUS FEA ( <a href="https://www.3ds.com/products-services/simulia/products/abaqus/">https://www.3ds.com/products-services/simulia/products/abaqus/</a> ) owned by Dassault Systemes, and Fast Fourier Transform solver AMITEX ( <a href="https://amitexfft.github.io/AMITEX/index.html">https://amitexfft.github.io/AMITEX/index.html</a> ) owned by CEA The DFT software VASP owned by VASP Software GmbH, <a href="http://www.vasp.at">www.vasp.at</a> (commercial license may be required).	
5	<b>Workflow and its rationale</b>	Micromechanics is the mesoscopic material modelling approach for revealing microstructure-property relationships. DFT provides data on microstructural and chemical stability of the alloy under a corrosive environment. The respective findings can be coupled to the micromechanical modeling to assess behavior at the scale of microstructure under corrosive environments.	



Table 3.2. Workflow

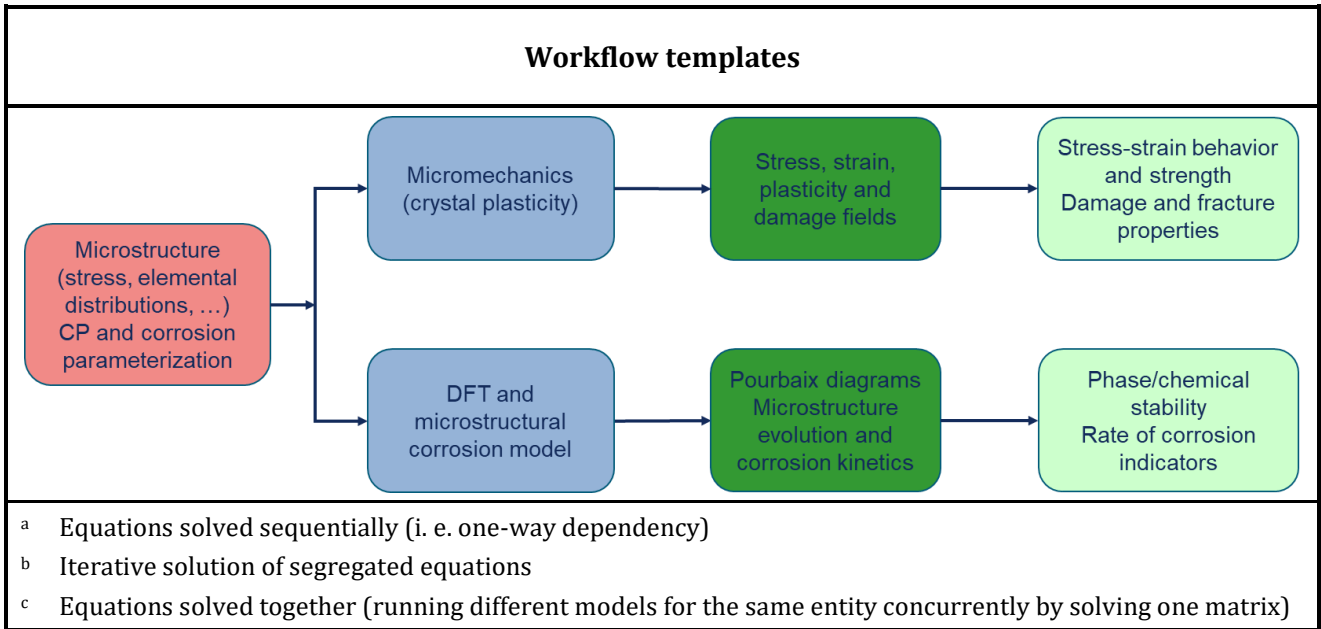




Table 3.3. Aspect of the user case / system to be simulated

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 1</b>	The multiscale material modelling workflow aims to understand microstructure-property relationships of high-entropy alloys manufactured by thermal spray coating. To this end, 2 modelling approaches are applied. Firstly, the microstructure of the coating either obtained from characterisation or simulation (grain geometry, crystallographic texture, elemental distribution, etc.) will be coupled with crystal plasticity model to perform a micromechanical simulation (model1) accordingly to predict mechanical performance. In parallel, DFT will be used to address phase stability in specific corrosive conditions.
1.2	<b>Material</b>	High Entropy Alloys (HEA) with 5-6 principal elements with or without hard metallic inclusions.
1.3	<b>Geometry</b>	The geometry of the system will be equivalent to the representative microstructural domain.
1.4	<b>Time lapse</b>	Time lapse is equivalent to the experimental references that modelling workflow aims to mimic.
1.5	<b>Manufacturing process or in-service conditions</b>	All in-service conditions will be taken into account as initial and boundary conditions for the modelling workflow.
1.6	<b>Publication on this data</b>	Not yet available



Table 3.4. Governing equations

2		Governing equations	
2.1	<b>Model type and name</b>	Micromechanics/Solid mechanics	
2.2	<b>Model entity</b>	The entity in this physics-based model is continuum volume.	
2.3	<b>Physics equation</b>	Equation	Plastic velocity gradient: $L^P = \sum_{s=1}^N \dot{\gamma}^s m^s \otimes n^s$ With: $\dot{\gamma}^s = f(\tau^s, \rho, T)$
		Physics quantities	$L^P$ : plastic velocity gradient, $\dot{\gamma}^s$ : slip rate, $m^s \otimes n^s$ : slip system, $\tau^s$ : shear rate, $\rho$ : dislocation densities, $T$ : temperature
2.4	<b>Materials relations</b>	Relation	Plastic velocity for describing the deformation is equal to the sum of slip rate of all slip system. The slip rate is calculated from the function explicitly considering shear rate, dislocation density, and temperature as the state variables.
		Physics quantities for each materials relation	Plastic velocity gradient, slip rate, slip systems, shear rate, dislocation density, and temperature
2.5	<b>Simulated input</b>	<ul style="list-style-type: none"> <li>- Microstructure obtained from characterisation or simulation.</li> <li>- All relevant material parameters including crystal plasticity parameters.</li> </ul>	



Table 3.5. Solver and computational translation of the specification

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	Finite element and Fast Fourier Transform solver	
3.2	<b>Software tool</b>	FE solver: <ul style="list-style-type: none"> <li>- Z-set (<a href="http://www.zset-software.com/">http://www.zset-software.com/</a>)</li> <li>- ABAQUS FEA (<a href="https://www.3ds.com/products-services/simulia/products/abaqus/">https://www.3ds.com/products-services/simulia/products/abaqus/</a>),</li> </ul> Fast Fourier Transform solver: <ul style="list-style-type: none"> <li>- AMITEX (<a href="https://amitexfftp.github.io/AMITEX/index.html">https://amitexfftp.github.io/AMITEX/index.html</a>)</li> </ul>	
3.3	<b>Time step</b>	Depending on the convergence study aiming at obtaining the most accurate results with the largest possible time step.	
3.4	<b>Computational representation</b>	Physics equation	Similar to the basic equation described in 2.3
		Material relations	Similar information provided in 2.4
		Material	Digitalised microstructure with all material parameters assigned.
3.5	<b>Computational boundary conditions</b>	Periodic micromechanical model with periodic boundary conditions to simulate an infinite domain	
3.6	<b>Additional solver parameters</b>	Numerical parameters to control the numerical efficiency of the solver may be adjusted depending on particular conditions.	



Table 3.6. Post-processing

4 Post-processing		
4.1	<b>The processed output</b>	The planned micromechanical simulations aim to predict mechanical behaviour of high entropy alloy coatings including: <ul style="list-style-type: none"><li>- Stress-strain behaviour</li><li>- Elastic modulus</li><li>- Strength</li><li>- Ultimate tensile strength</li><li>- Failure strain.</li></ul>
4.2	<b>Methodologies</b>	Micromechanical simulation results will be homogenised using the volume averaging method to predict macroscopic mechanical properties.
4.3	<b>Margin of error</b>	Maximum 5% deviation from experimental reference.



Table 3.7. Aspect of the user case / system to be simulated for model 2

1	Aspect of the user case / system to be simulated	
1.1	<b>Aspect of the user case to be simulated using model 2</b>	Computational screening of Pourbaix diagrams to investigate the suitability of selected alloy chemistries to operating under corrosive environments.
1.2	<b>Material</b>	High Entropy Alloys (HEA) and High Entropy Carbides (HEC) with 5-6 principal elements or less.
1.3	<b>Geometry</b>	Lattice, supercell
1.4	<b>Time lapse</b>	Equilibrium state calculations
1.5	<b>Manufacturing process or in-service conditions</b>	Solution chemistry of the corrosive environment, described via activities and concentrations of the species and ions critical for the degradation mechanisms.
1.6	<b>Publication on this data</b>	Not yet available.

Table 3.8. Governing equations, model 2

2	Governing equations		
2.1	<b>Model type and name</b>	Density functional theory (DFT)	
2.2	<b>Model entity</b>	The entity in this physics-based model is electron.	
2.3	<b>Physics equation</b>	Equation	Electronic Schrödinger equation: $\hat{H}\Psi = [\hat{T} + \hat{V} + \hat{U}] \Psi = \left[ \sum_{i=1}^N \left( -\frac{\hbar^2}{2m_i} \nabla_i^2 \right) + \sum_{i=1}^N V(\mathbf{r}_i) + \sum_{i<j}^N U(\mathbf{r}_i, \mathbf{r}_j) \right] \Psi = E\Psi,$
		Physics quantities	$\hat{H}$ is the Hamiltonian, E is the total energy, T is the kinetic energy, V is the potential energy from the external field due to positively charged nuclei, and $\hat{U}$ is the electron–electron interaction energy.
2.4	<b>Materials relations</b>	Relation	Wavefunction satisfying the many-electron Schrödinger equation.
		Physics quantities for each materials relation	Elemental chemistry of a certain structure and phase.
2.5	<b>Simulated input</b>	Candidate material chemistries are utilized as input.	



Table 3.9. Solver and computational translation of the specification for model 2

3		Solver and computational translation of the specifications	
3.1	<b>Numerical solver</b>	ab initio quantum mechanical solver	
3.2	<b>Software tool</b>	VASP ( <a href="http://www.vasp.at">www.vasp.at</a> )	
3.3	<b>Time step</b>	Not applicable.	
3.4	<b>Computational representation</b>	Physics equation	See 2.3.
		Material relations	Projector augmented wave, plane wave basis set, pseudopotentials
		Material	Functionals, potentials
3.5	<b>Computational boundary conditions</b>	Unit cell with periodic boundary conditions, surfaces, interfaces.	
3.6	<b>Additional solver parameters</b>	Solver parameters are incorporated and adjusted depending on particular analysis needs.	

Table 3.10. Post-processing for model 2

4		Post-processing
4.1	<b>The processed output</b>	Pourbaix diagrams.
4.2	<b>Methodologies</b>	Post-processing scripts will be developed during the course of the work.
4.3	<b>Margin of error</b>	Not applicable.



## 4 ML Modelling

### 4.1 ML Modelling of HEA and Microstructures

ML model developed for the CoBRAIN project.

Model owner [AEONX AI, [marzuk.kamal@aeonx.ai](mailto:marzuk.kamal@aeonx.ai) ]

Table 4.1. Overview of the ML Modelling

Overview of the ML modelling			
1	<b>User case</b>	ML Models to estimate physical properties of High Entropy Alloys/Hard Metals, modelling Microstructure, Modelling Alloy phases, Development of ML Surrogate Models	
2	<b>Model Types</b>	Model 1	Graph Neural Networks
		Model 2	Fully connected Neural Networks
		Model 3	Graph Neural Network with Exploitability through transformers and SHAPLEY methods.
3	<b>Publication peer-reviewing the data</b>	Not yet available.	
4	<b>Access conditions</b>	ML Models will be built using TensorFlow and/or PyTorch. TensorFlow and PyTorch are open-source ML frameworks that is maintained by Google and Facebook respectively. Models will be deployed as REST API, which is build using FastAPI web framework and Python/Dask distributed computing framework.	
5	<b>Workflow and its rationale</b>	Graph Neural Network and Transformer based models are effective ML architectures to study microstructure properties and phase of Alloys .	



## 5 Baselines for computing hardware

The different simulation tools utilized in the workflows above have all different requests for computing hardware and data storage, hence they do not run all together on a single computer. This requires dedicated solutions for the interoperability between the different models.

The partners are developing and operating different solutions in terms of so called “simulation platforms”, in particular the AixViPMaP platform [Ref1] from ACS or properTune from VTT. “Simulation platforms” can be considered as a software toolbox which enables the implementation of a workflow in a “real” computing hardware environment. The simulation platform provides certain services for the orchestration of individual simulation runs in a heterogeneous computing network, it supports and provides data format converters which are needed for the data exchange between the different models and additionally offers interfaces for the data transfer via different kinds of cloud resources. Furthermore, it integrates also pre- and postprocessing tools.

The workflow “MATERIAL” as defined in the MODA will be implemented on the AixViPMaP platform at the partner ACS. On the AixViPMaP a workflow is utilized via so called Jupyter notebooks which comprise also the pre- and postprocessing work associated with the workflow. A solution for the integration of the DFT computations which will run on computers outside the network of ACS needs to be developed and integrated in the CoBRAIN project.

A similar setting will be provided by VTT for the workflows PROCESS and PROPERTY based on their Integrated Computational Materials Engineering (ICME) concept Propertune which facilitates interactions between computational tools and execution of high-throughput workflows.

[Ref1] L. Koschmieder, S. Hojda, M. Apel, R. Altenfeld, Y. Bami, C. Haase, M. Lin, A. Vuppala, G. Hirt, G. J. Schmitz, „AixViPMaP - an Operational Platform for Microstructure Modeling Workflows”, Integrating Materials and Manufacturing Innovation, Vol. 8 (2), pages: 122-143, DOI: 10.1007/s40192-019-00138-3



## 6 Conclusions

MODAs have been developed for the main modelling approaches employed in the project, further divided into computational compositional screening, process modelling, and properties' modelling methods. These workflows reflect the ongoing activities of WP2 and will also help ensuring the accessibility and interoperability among the various modelling procedures. Thus, they are an essential basis for the future development of AI models on their basis. To this end, the deliverable also contains a section dedicated to the integration among the various models and the related hardware requirements.

Finally, the combination of fully documented modelling and characterization workflow (deliverable 1.3) will facilitate the discover of potential new relationships between properties. This integration can thus produce new knowledge, and it can generate business opportunities, complementing the extant industrial standards.



## 7 Attainment of Objectives

Table 7.1. Contribution to the general objectives of CoBRAIN

Ref. <sup>3</sup>	General Objective	Status
O2.2	<b>CHADA workflow for clear understanding of the composition-process-microstructure-properties- performance correlation chain</b>	This deliverable does not contribute directly to the implementation of the CHADAs workflows but supported the identification of the characterization methods which can better validate the models
O2.3	<b>MODA workflow for a comprehensive computational description of the coating performances</b>	This document constitutes the MODA workflow as foreseen in the project, including workflows for specific characterization methods defined in accordance with CWA17284 as well as overall workflows used to orchestrate the various models in the ICME platform AixVIPMaP.
O2.4	<b>Machine learning architecture capable of driving the materials development for multicomponent alloys to deliver application-specific metal coating properties</b>	This deliverable does not contribute directly to the definition of a machine learning architecture but gives indication on the modelling framework which will be utilised by the algorithms.

Table 7.2. Contribution to the specific workpackage objectives

Ref. <sup>4</sup>	Work Package Objective	Status
WP1.1	To Specify a complete MODA and CHADA to be used in the project	This deliverable provides the complete MODA to be used in the project
WP1.3	To Create a set of ontological relations that connect and describe Modelling, Characterization and TS processes	The ontological relations are being prepared in parallel and in compliance with the definition of MODA and CHADA.
WP1.2	To Create an OWL-DL ontological representation of the manufacturing processes	Not directly related to this deliverable. Activities are progressing as planned.
WP1.4	To Store everything in a Knowledge Base repository exploiting commercially available RDF Triplestore	Not directly related to this deliverable. Activities are progressing as planned.

<sup>3</sup> Reference to the general project objectives stated from page 4 of Part B of the Annex 1 – Description of Action

<sup>4</sup> Reference to the specific objectives of the workpackage as listed in Part A of Annex 2 – Description of Action