Neuro – symbolic AI for materials modelling and processes design

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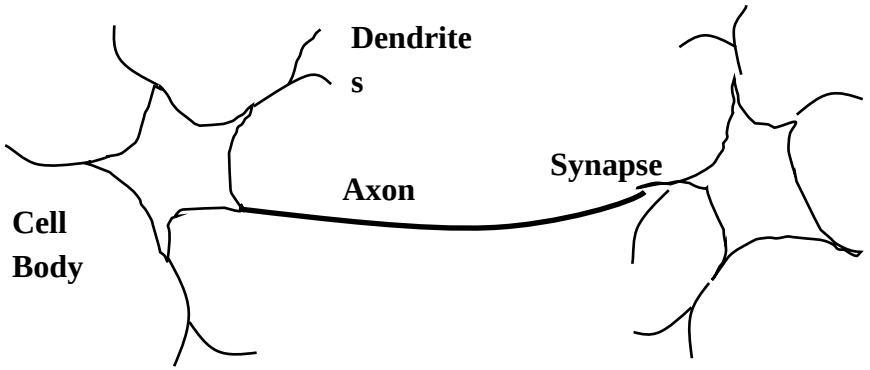
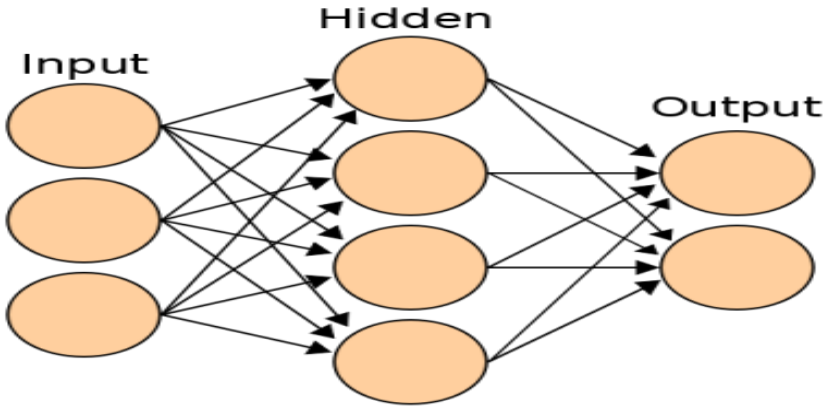
Artificial Neural Networks (ANNs):

- **Inspired from biological neurons**
- **Trained with data** (e.g. experimental data, historical data)
- **Can represent Multi-input and Multi-output models**

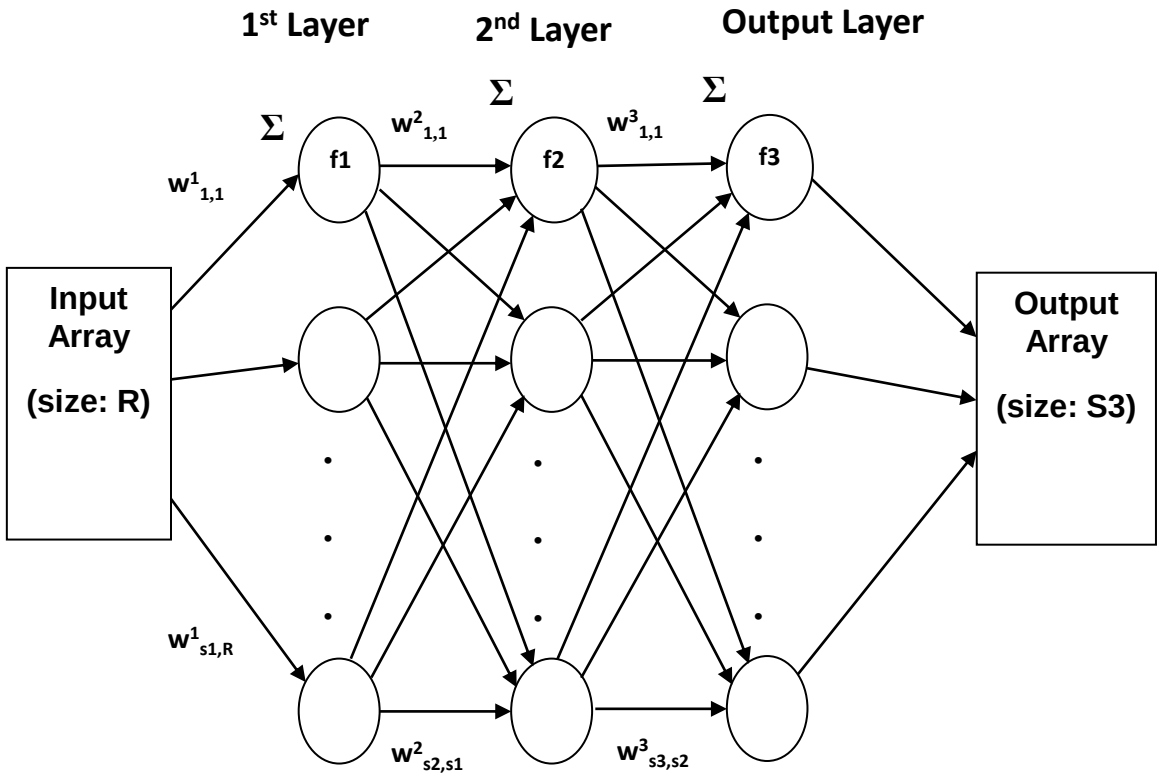


Basic structure of biological neurons



Artificial Neural Network

Structure of the Multi-Layer Perceptron (MLP) ANN:

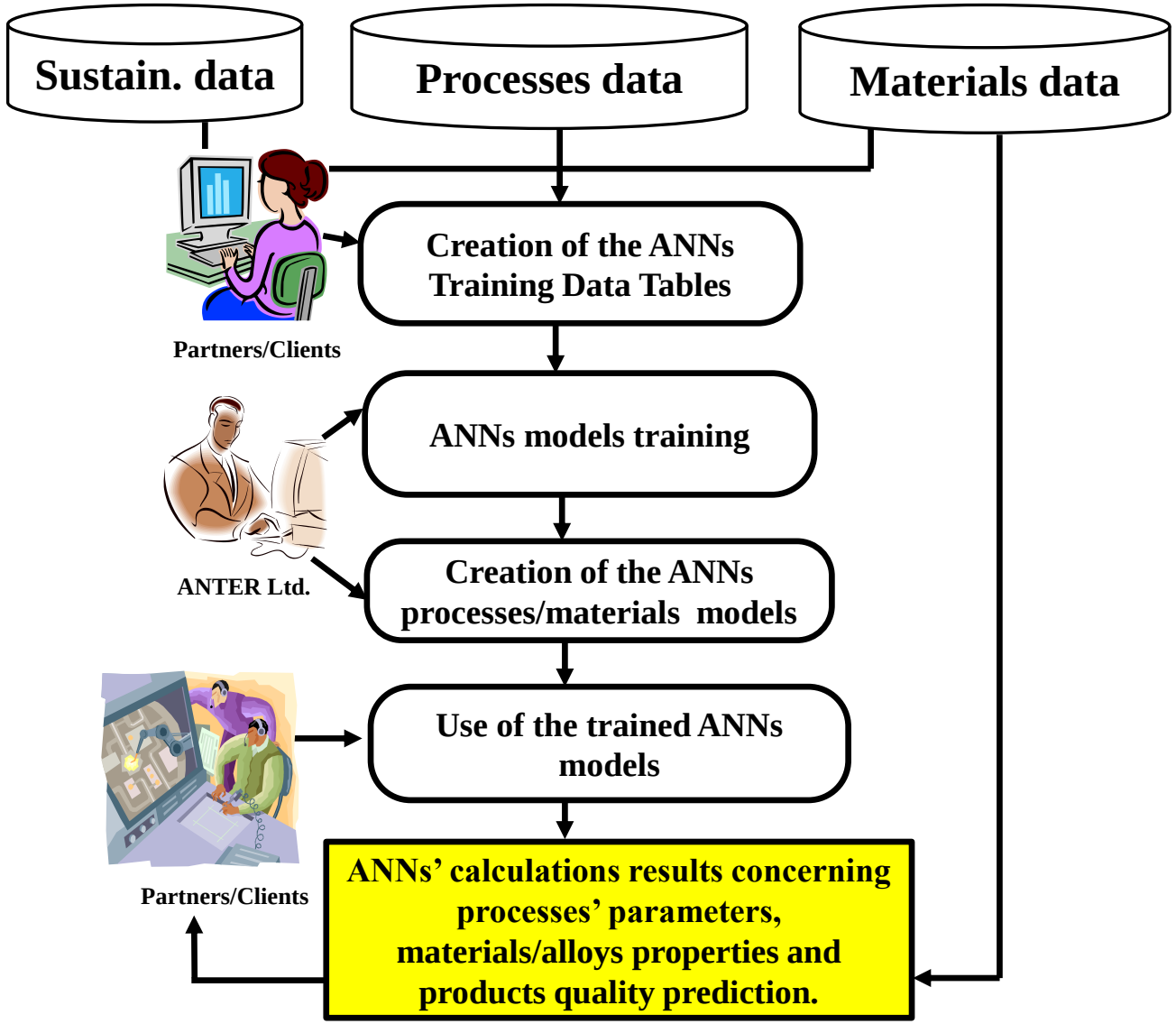


Multilayer Perceptron (MLP) Feed forward (R-S1-S2-S3) ANN with 2 hidden layers of neurons

- **MLP ANNs are often used for Function approximation and for the Modelling of processes, systems, materials, etc.**

Artificial Neural Networks (ANNs):

- **ANNs can be useful when mathematical and physics-based models are missing or are not applicaple, e.g. in cases of:**
  - **new** processes,
  - **new** material alloys,
  - **new** products,
  - etc.



Symbolic AI

- Includes Rule-based and Object-Oriented (O-O) methods for Knowledge representation and processing (Knowledge Based Systems - KBS).

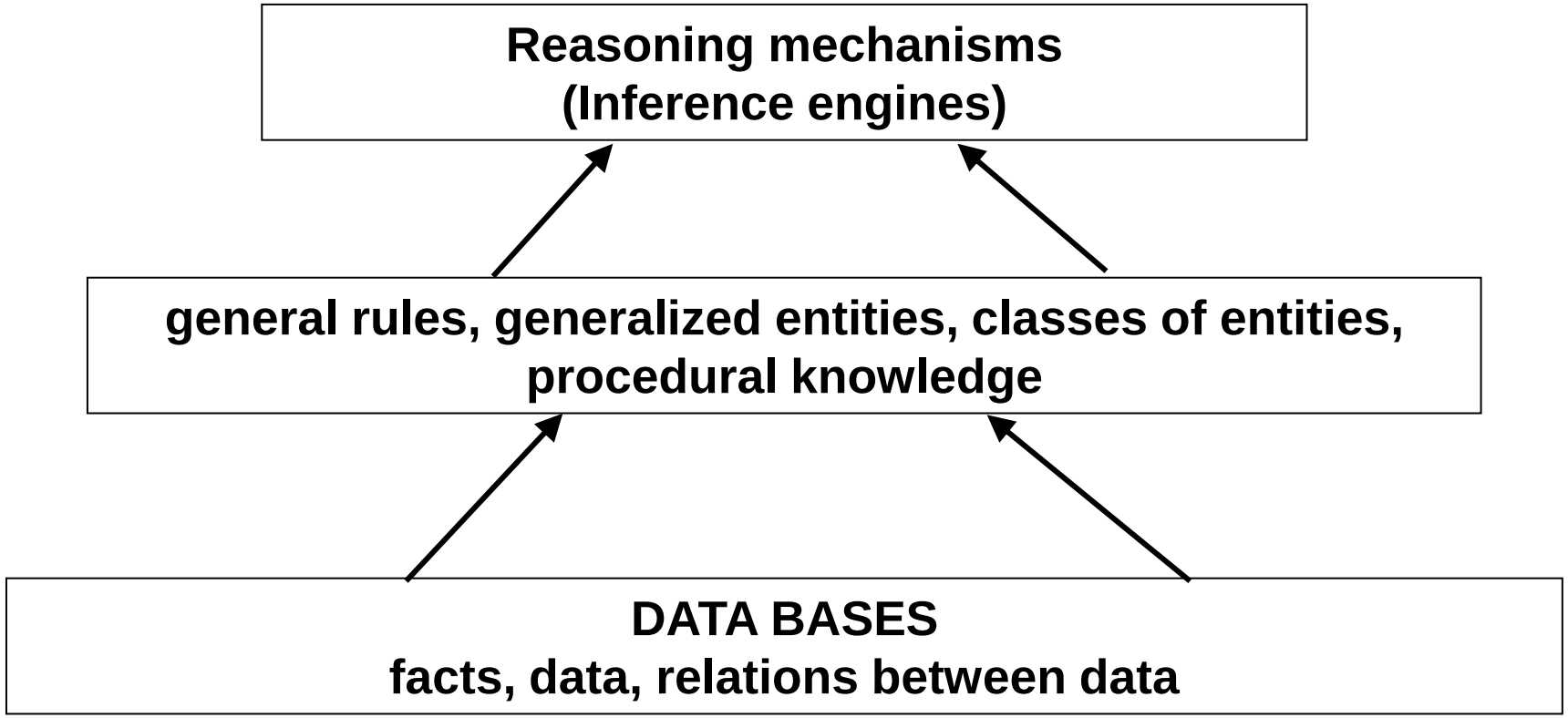
- Knowledge Representation Structures (KRS) used:
  - Rules
  - O-O structures
    - Semantic Networks
    - Frames / Objects

Symbolic AI - Knowledge Based Systems (KBS):

- **The knowledge processing methods (e.g. for reasoning) are based on the Knowledge Representation Structures (KRS) used, and more specifically:**
  - For **Rule-based** structures:
    - **Backward** and **forward** chaining of rules.
  - For **Object-Oriented** structures (Semantic networks, Frames/Objects):
    - Inferences about **existence of entities and their attributes**, inferences for **generic and default properties**, inferences **by analogy**, etc.

Symbolic AI - Knowledge Based Systems (KBS):

- **Knowledge Classification**



In summary

Symbolic AI methods & Knowledge Based Systems (KBS):

- Originate also from AI research.
- Use formal methods for knowledge representation and processing (Rule-based, Object-Oriented).
- Can include reasoning mechanisms (inference engines).
- Can be used for the representation, storage and processing of human knowledge and experience.
- Can support human decision-making.
- Can work in parallel with mathematical models, algorithms and data-driven AI methods (e.g. ANNs).

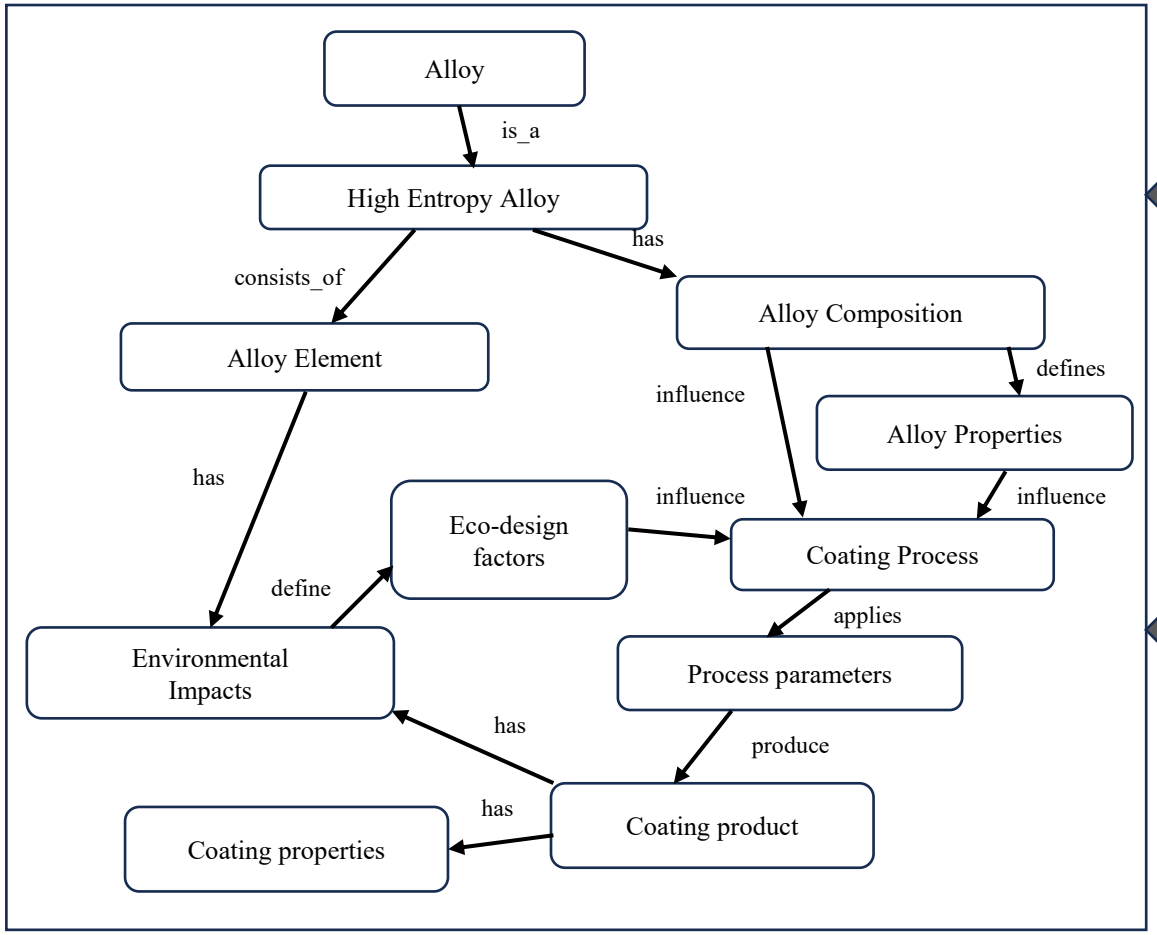
Symbolic AI – KBS & Ontologies:

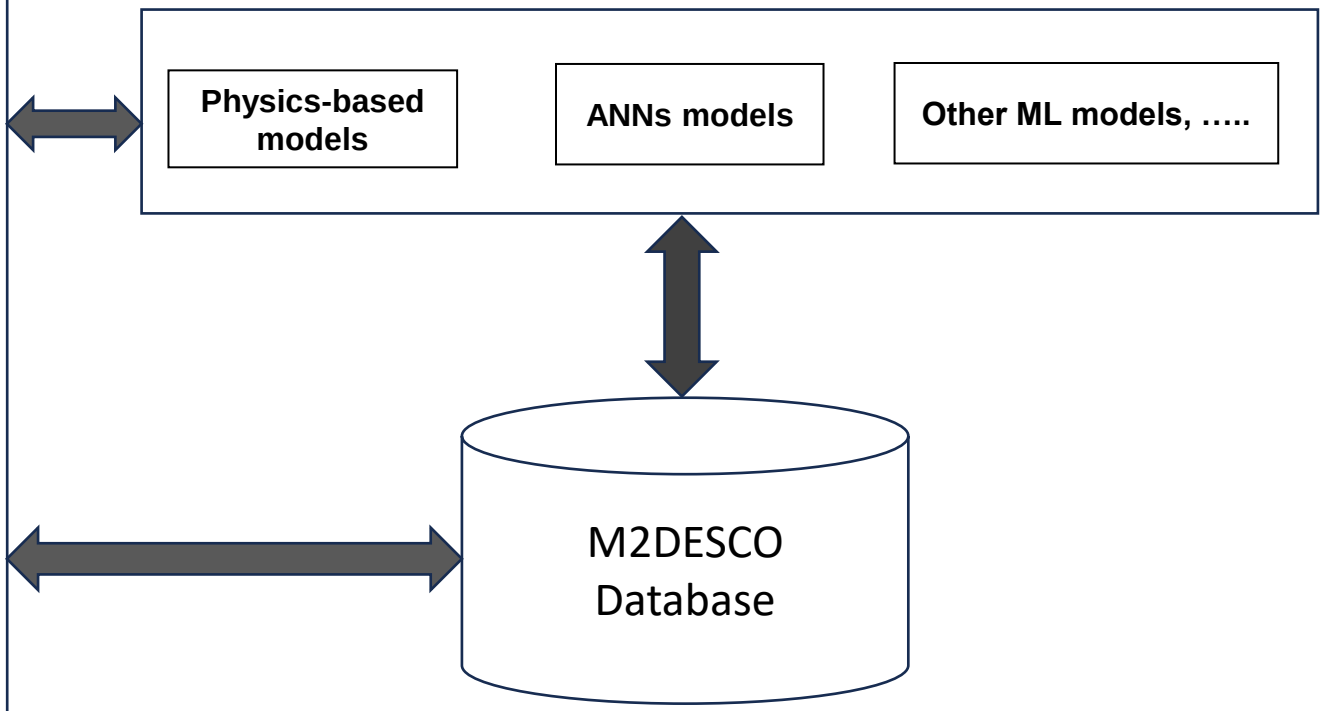
- **Even though lately in the Semantic Web community, the term "Ontologies" is being used instead of the term "KBS", the main principles of Knowledge Engineering for KBS are applied also for the development of Semantic Web Ontologies [6, 7]. In fact, Ontologies can be considered as a combination of the above-described rule-based and O-O KRS and more specifically [8]:**

- ***Ontology = < taxonomy, inference rules >, where***
- ***Taxonomy = < {classes}, {relations} >.***

Symbolic AI – Semantic Network example:

- **Semantic entities' relations of High Entropy Alloys' (HEAs) coatings**





Benefits of integrating ANNs with Symbolic AI (Neuro-symbolic AI):

- Improving ANNs modelling accuracy by applying **ANNs' training optimization rules.**
- Design of materials/products using **eco-design rules combined with ANNs predictions** on Sustainability & Life Cycle Analysis.
- **Reasoning on manufacturability** of products/materials and **environmental impacts** of processes & materials.
- **Prediction and reasoning on quality properties** and **identification of causes of bad quality.**
- **Representing and updating materials modelling ontology** (e.g. as proposed by the EMMC MODA framework) using materials science theory, expert human knowledge and physics-based or ANNs models results.

Thank you !!

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