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TOWARDS DIGITALIZATION AND HYBRID MODELING IN MATERIAL RESEARCH

MICHAEL DOGGE

MICHAEL.DOGGE@BOSCH.COM

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Background – Bosch Vision

To comply with the Bosch and PS-CT vision there is a need for even deeper understanding of materials and their behavior, which dictates process requirements and product performance.

Integrating AI methods can make this possible!

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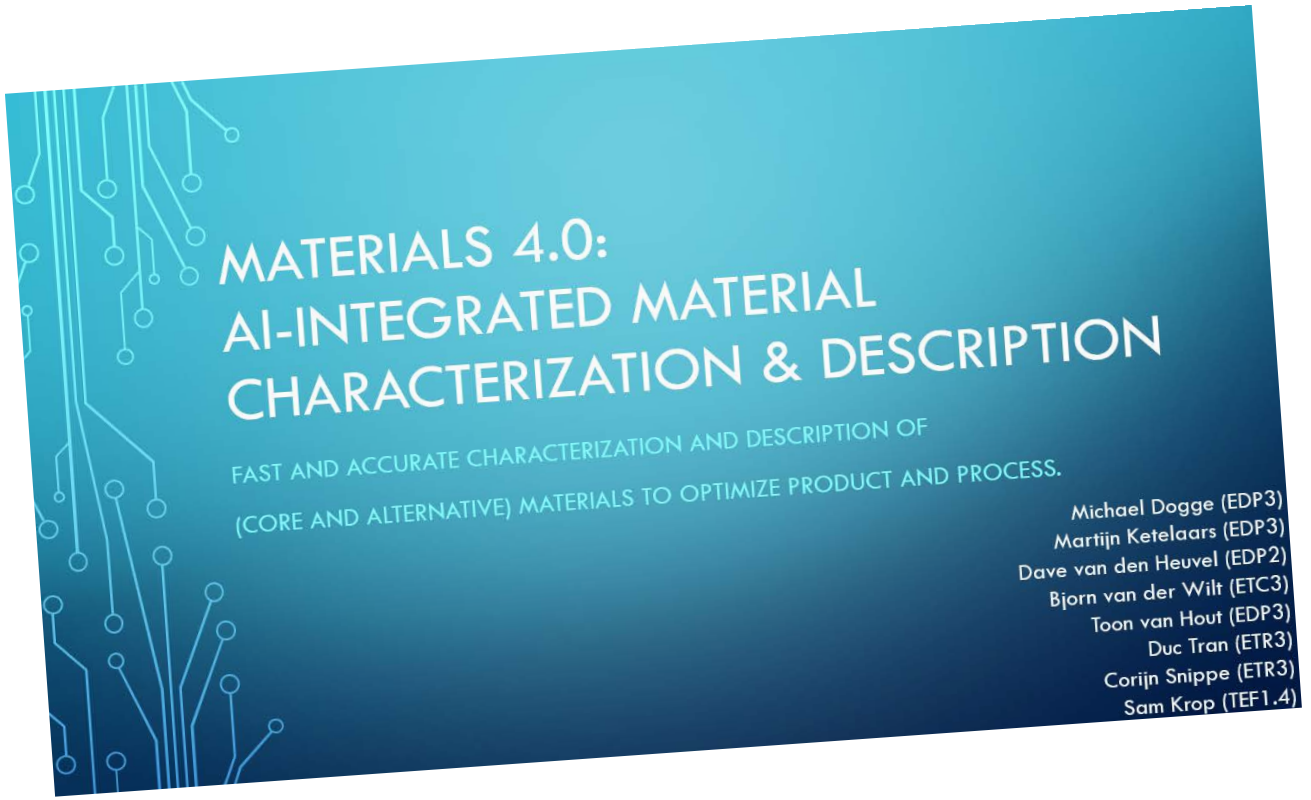
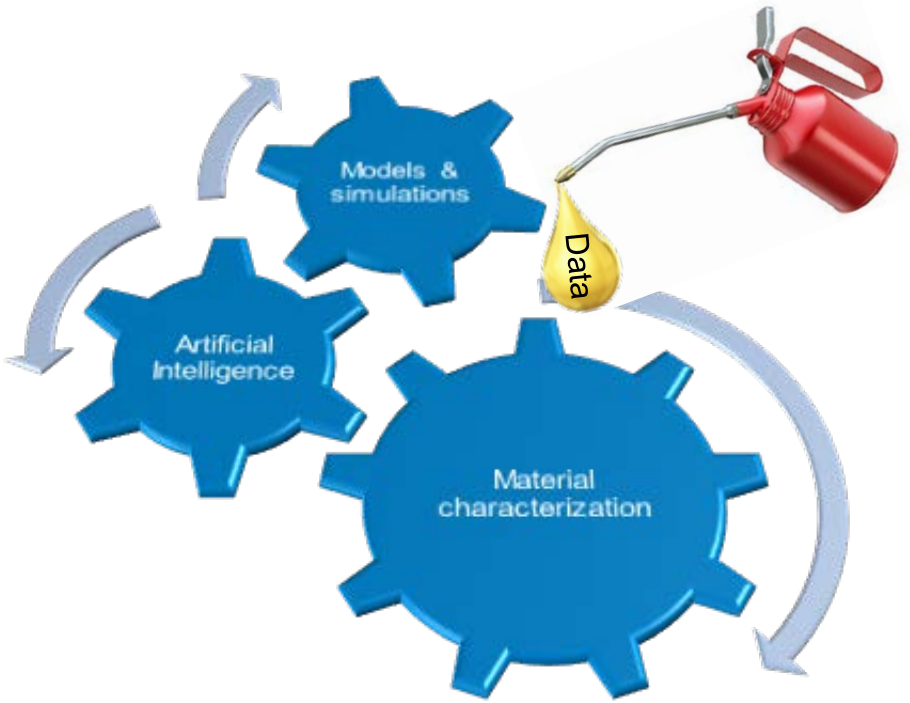
Introduction Materials 4.0[*] project

- Project launched for advanced material characterization using “state-of-art” concepts.





[*] Rajan Jose, Seeram Ramakrishna, *Materials 4.0: Materials big data enabled materials discovery*, https://doi.org/10.1016/j.apmt.2017.12.015.

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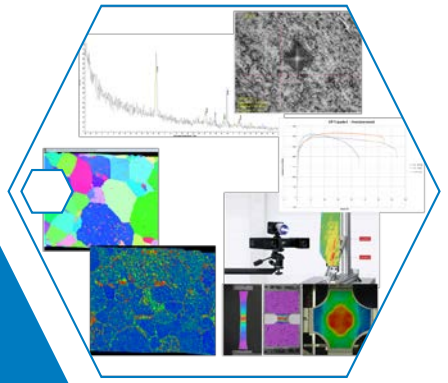
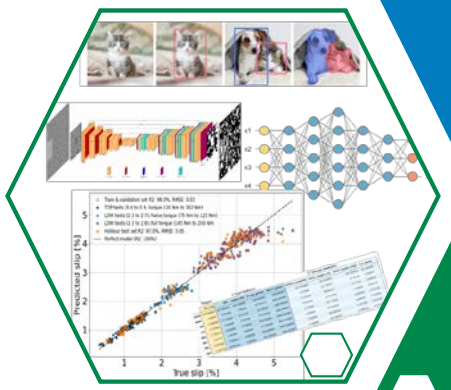
Overview activities



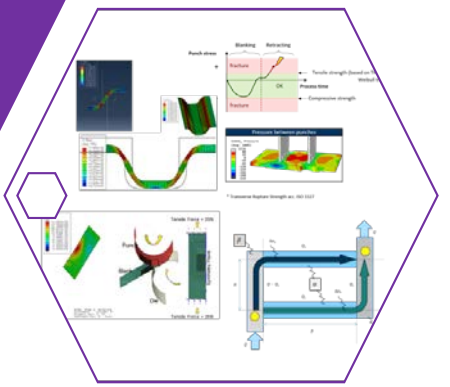
Material characterization

Characteristics of microstructure
Composition of material
Behavior & anisotropy
Forming limits



Model and simulations

Optimization of product and process
Generate engineering relations
Accurately apply know-how
Explore new solutions



Artificial intelligence

Faster analysis
Explore new solutions
Collect new types data
Advanced handling & interpret data

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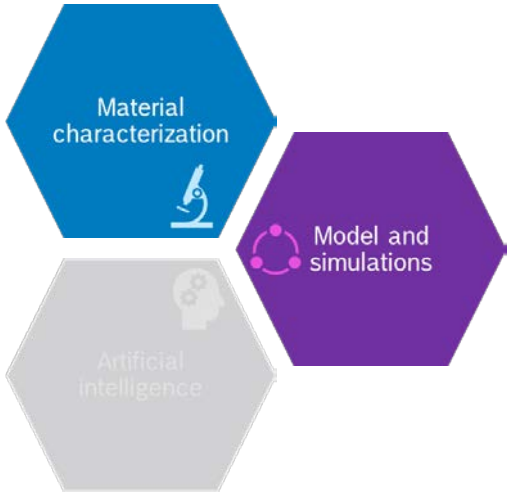
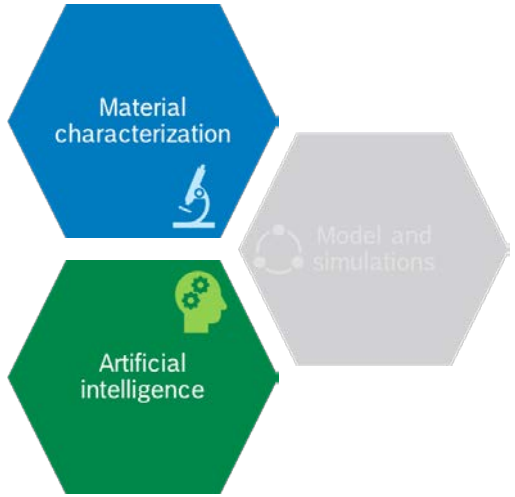
Research topics

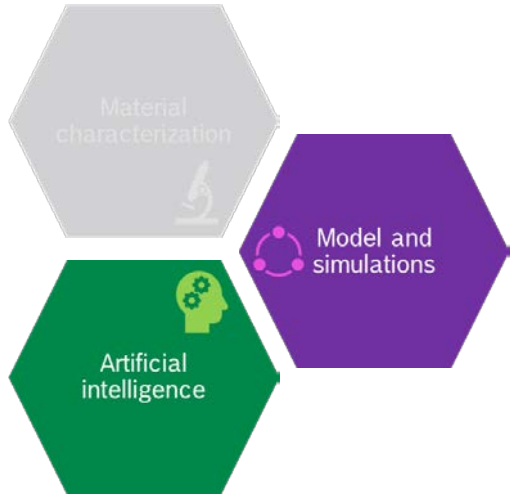


- “Classical” experimental-numerical analysis
- Model fitting with experiments
- Parameter estimation on measurement data
- (Advanced) material modeling



Example 1a: Deep learning SEM analysis

Example 1b: Predict key material properties



Example 2a: Neural network RVE integration

Example 2b: Hybrid material modeling

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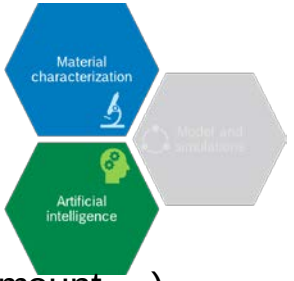
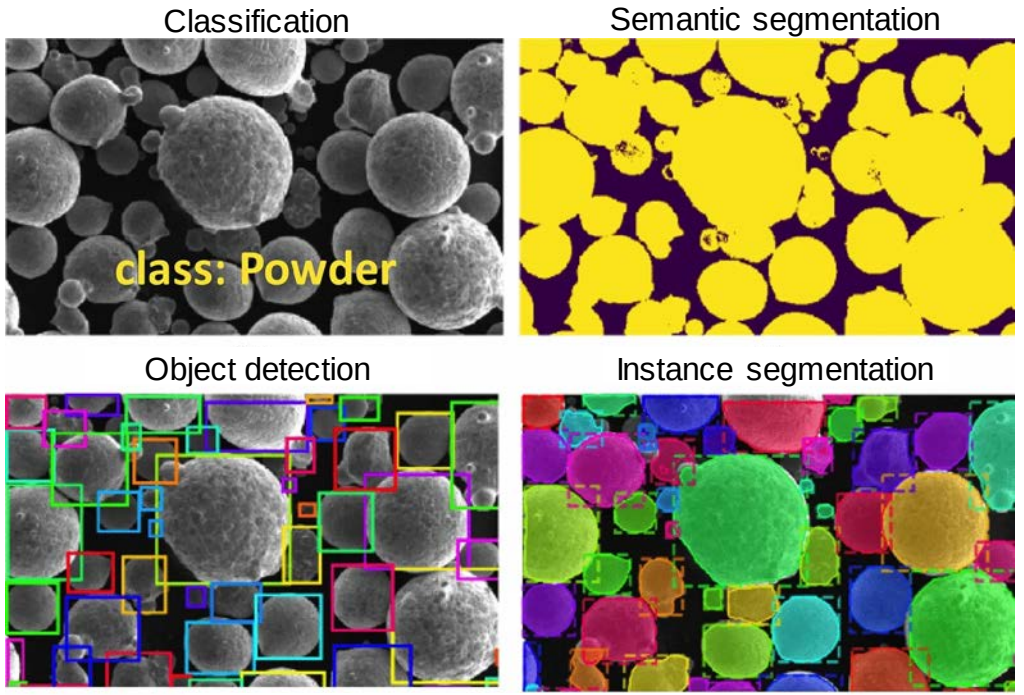
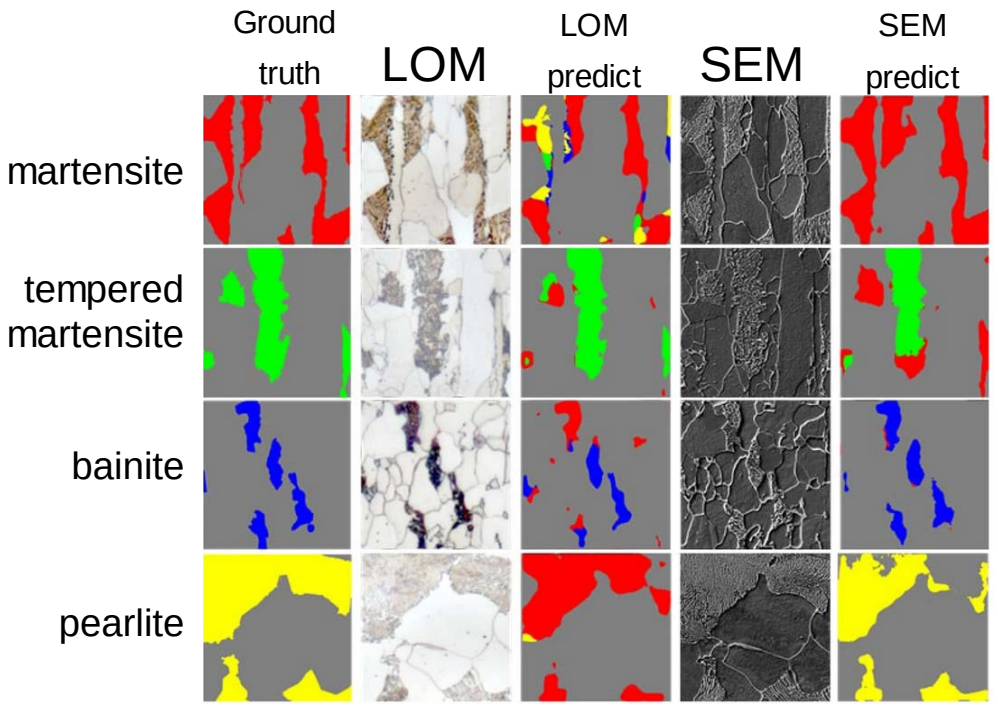
1a) Deep learning SEM analysis



- Goal: Robust way to extract more, and more accurate quantitative microstructure data (E.g., volume, shape, size, amount,…).



FROM: Holm, E.A., Cohn, R., Gao, N. et al. Overview: Computer Vision and Machine Learning for Microstructural Characterization and Analysis. Metall Mater Trans A 51, 5985–5999 (2020). https://doi.org/10.1007/s11661-020-06008-4



*FROM: Azimi, S.M., Britz, D., Engstler, M. et al. Advanced Steel Microstructural Classification by Deep Learning Methods. Sci Rep **8**, 2128 (2018). https://doi.org/10.1038/s41598-018-20037-5*

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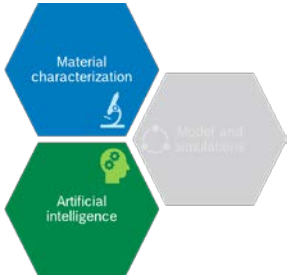
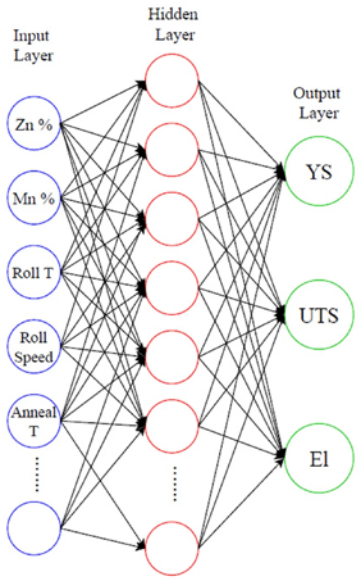
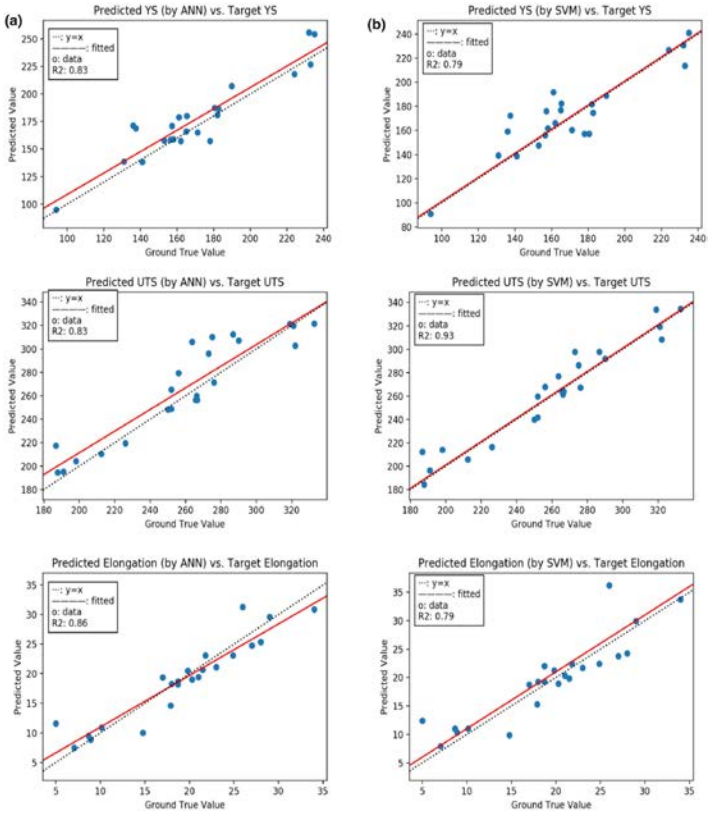
1b) Predict key material behavior



- Goal: Predict (key) material behavior based on “simple” material characteristics and properties.

composition	Composition of Zn (%)
	Composition of Al (%)
	Composition of Mn (%)
	Composition of Ca (%)
	Composition of Si (%)
process settings	Homogenization temperature (°C)
	Homogenization duration (h)
	Extrusion temperature (°C)
	Extrusion ratio
	Extrusion speed (mm/s)
	Rolling temperature (°C)
	Rolling reduction (%)
	Rolling speed (mm/s)
	Annealing temperature (°C)
	Annealing duration (h)
	Angle between loading and processing direction (°)
Results	Yield strength (MPa)
	Ultimate tensile strength (MPa)
	Elongation (%)





More examples:

- Anisotropy
- Forming limit
- Fatigue

*FROM: Xu, X., Wang, L., Zhu, G. et al. Predicting Tensile Properties of AZ31 MagnesiumAlloys by Machine Learning. JOM **72**, 3935–3942 (2020). https://doi.org/10.1007/s11837-020-04343-w*

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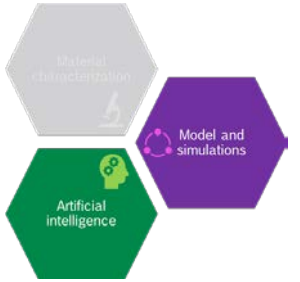
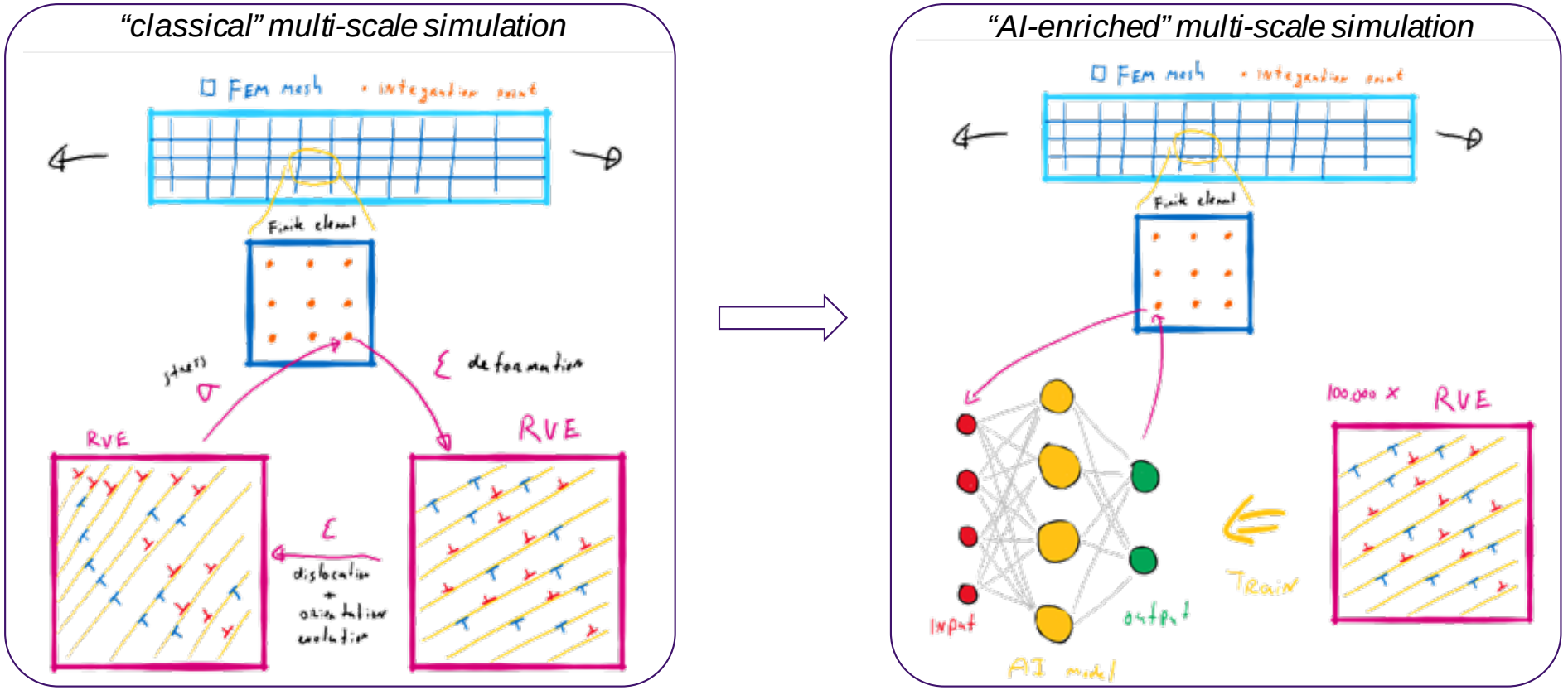
2a) Example 2a: Neural network RVE integration



- Goal: Efficiently enrich product & process simulations with underlying (microscale) physics to increase accuracy.



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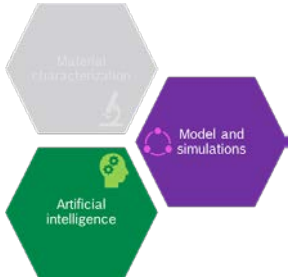
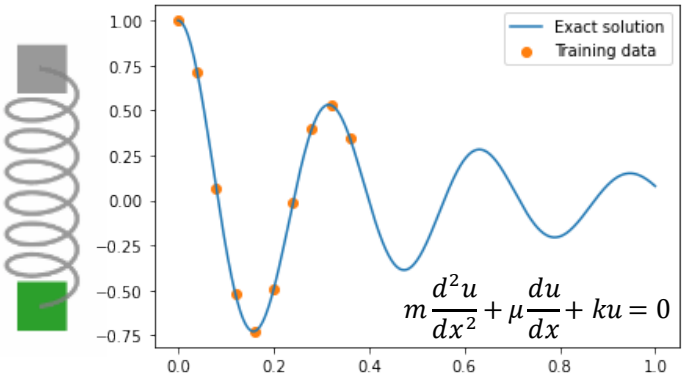
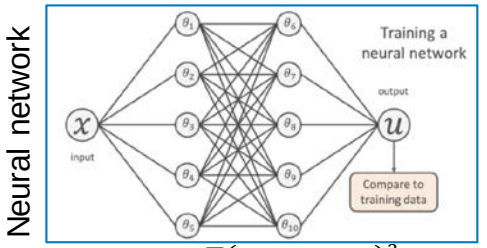
2b) Example 2b: Hybrid (material) modeling

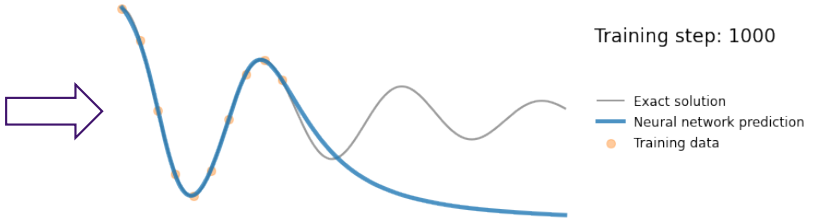


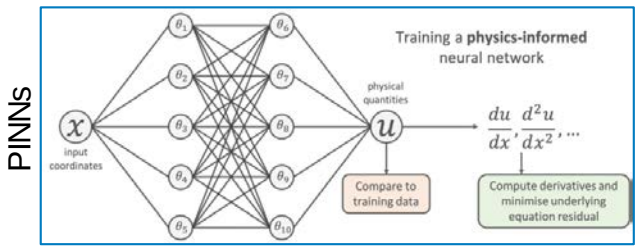
- Goal: Enrich data-driven AI neural network with known physics to increase predictability.
  - Physics Informed Neural Networks (PINNs)



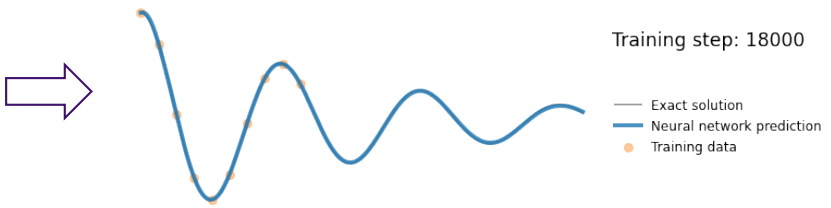


$$\min\sum(u_{NN}-u_{true})^2$$





$$\min\sum(u_{NN}-u_{true})^2+\sum\left(\left[m\frac{d^2}{dx^2}+\mu\frac{d}{dx}+k\right]u_{NN}\right)^2$$



Ref: https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

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Summary / outlook

- Use state-of-art characterization methods;
- Enrich models & simulations with proper and extended know-how.
- Integrate AI methods to:
  - Extract more information, faster;
  - Explore (non-trivial) relations and solutions;
  - Enrich numerical analysis for faster and more accurate predictions;