



The modern-day blacksmith

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About

Machine learning software to aid experimental design

Merge and aggregate all sources of data: experimental, computational, and analytical

Predictive models **reduce costs** and **accelerate discovery** process

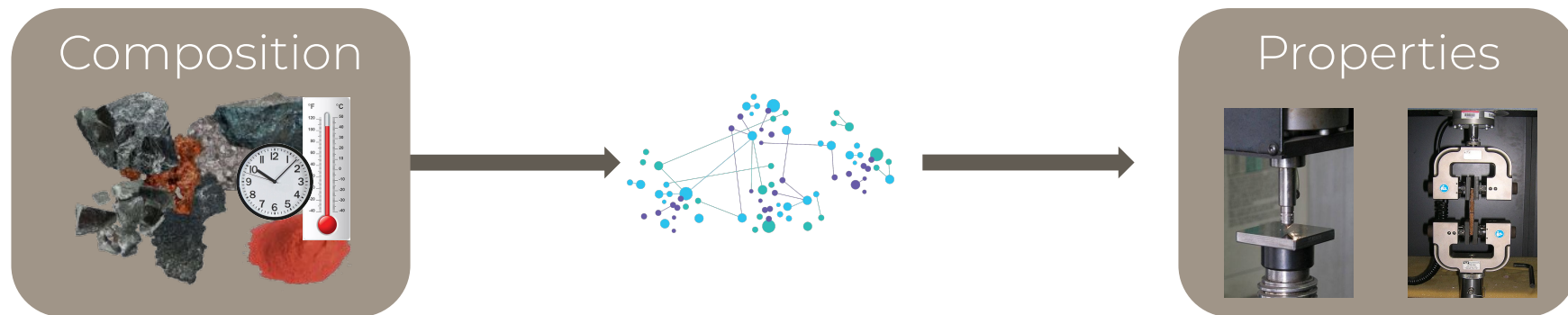
Traditional experimental design

Process is **expert driven**, subjective, and **iterative** through trial and improvement

Process takes ~20 years and specialist alloys cost >\$10m to develop, drugs cost >\$1bn

Standard machine learning

Standard algorithms exploit **composition-property** correlations



Alchemite™ machine learning on sparse data

Standard algorithms exploit **composition-property** correlations

Alchemite™ predicts from **available** inputs:
property-property correlations and computer simulations

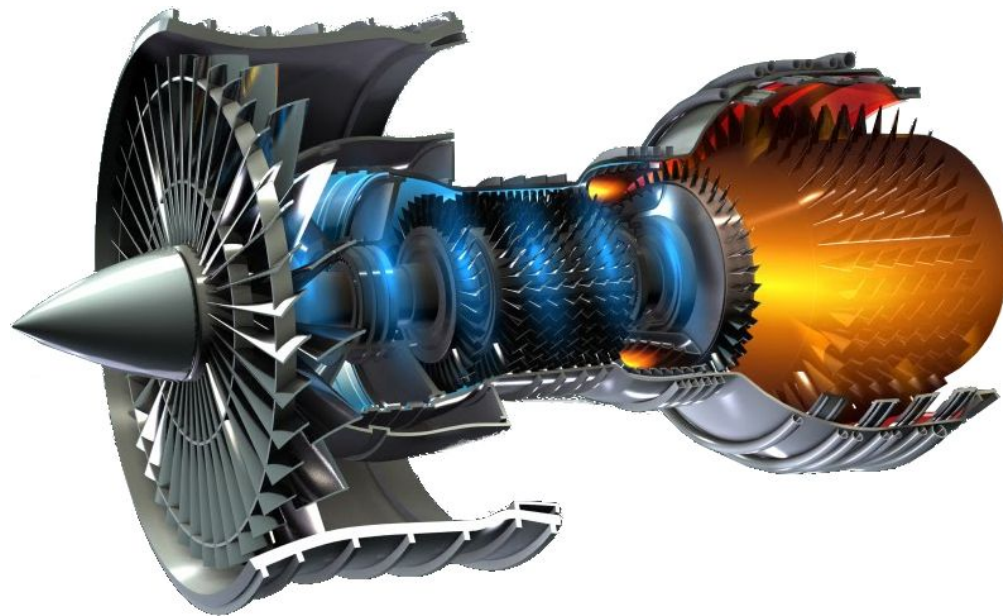
Typical experimental data is 0.2% complete so algorithm must handle **missing** data

Optimized design process

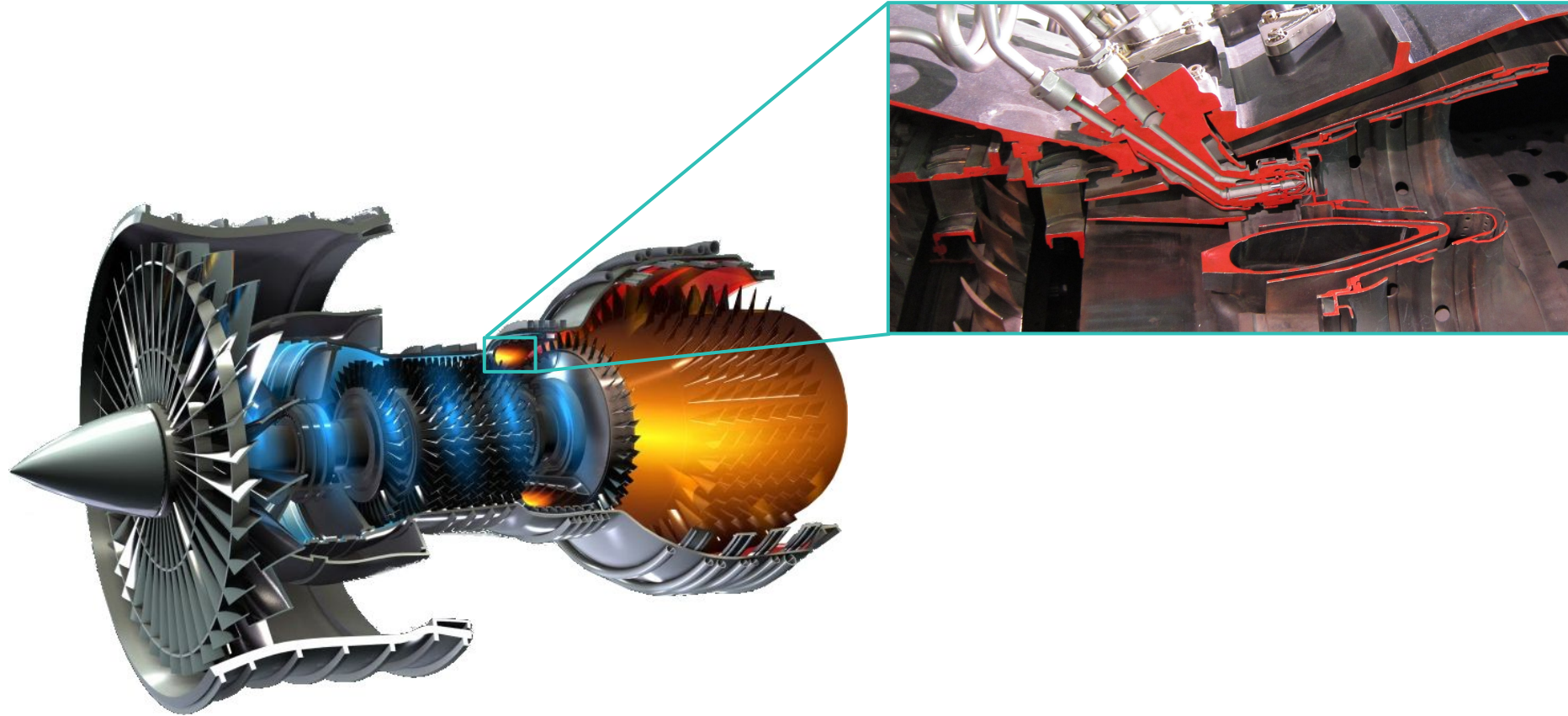
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

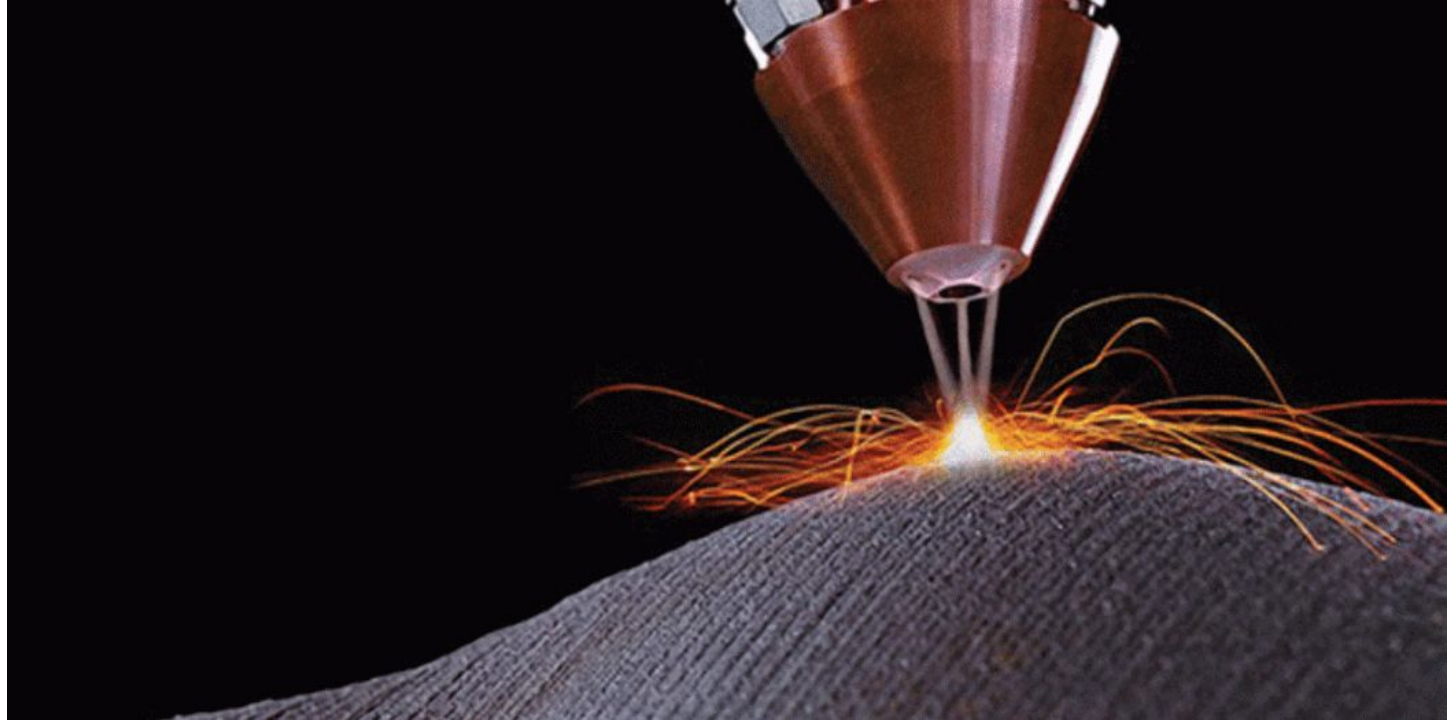
Schematic of a jet engine



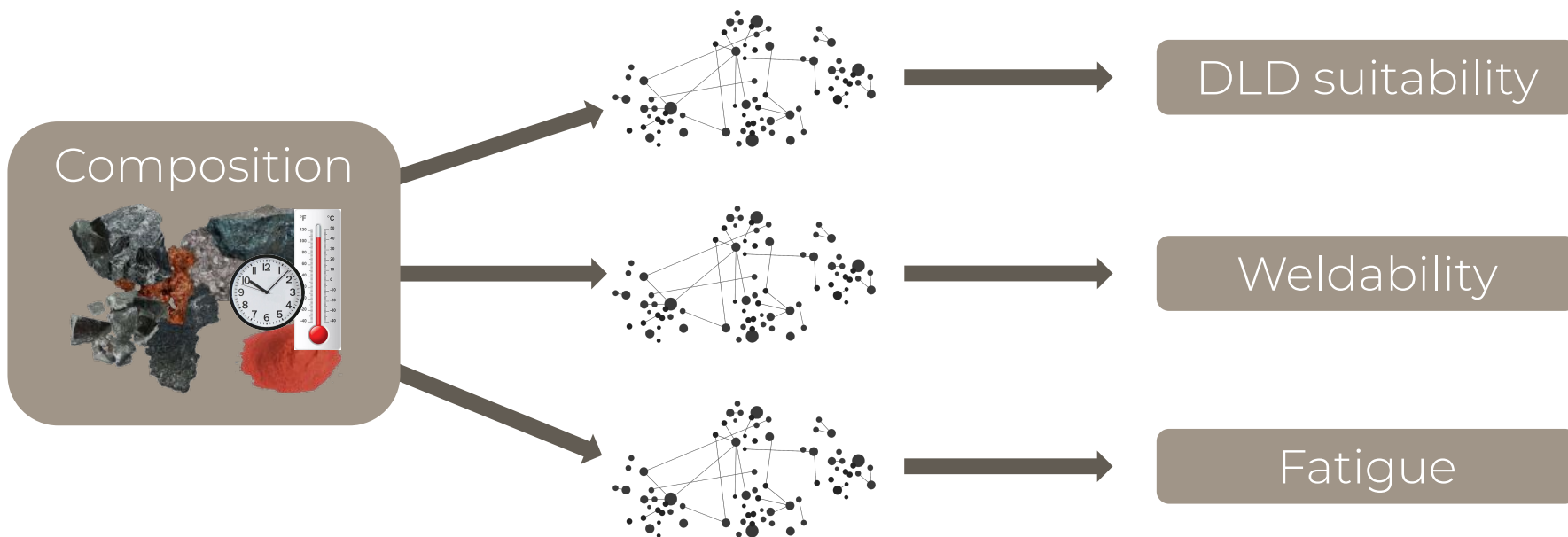
Combustor in a jet engine



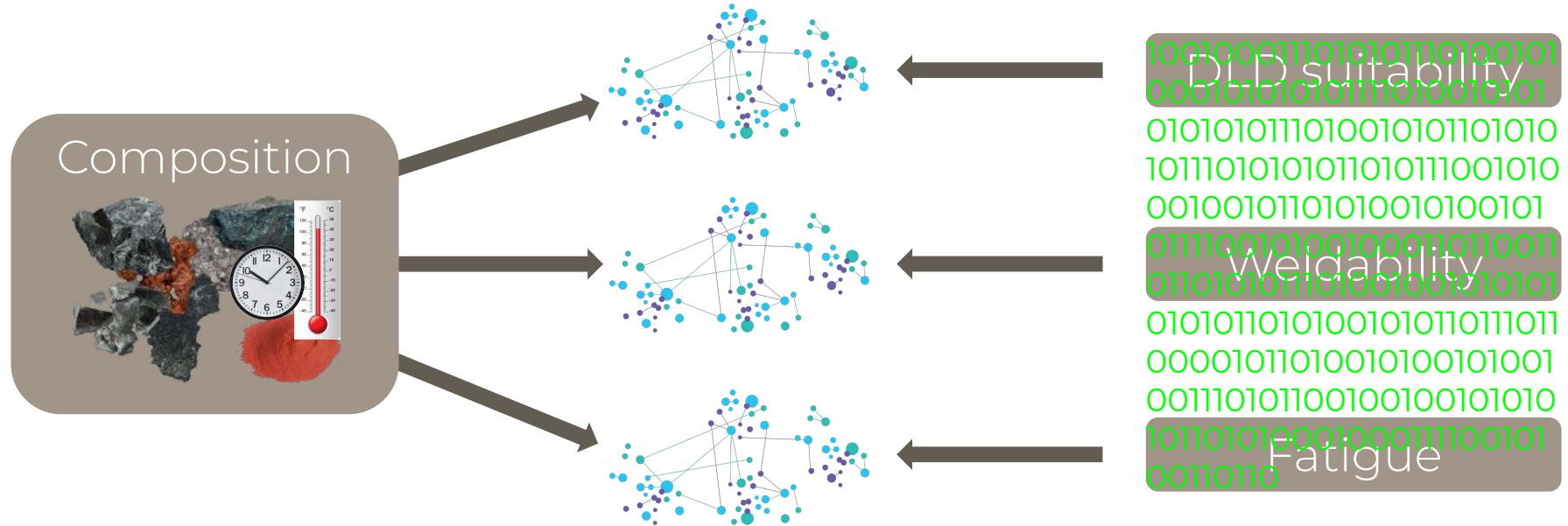
Direct laser deposition requires new alloys



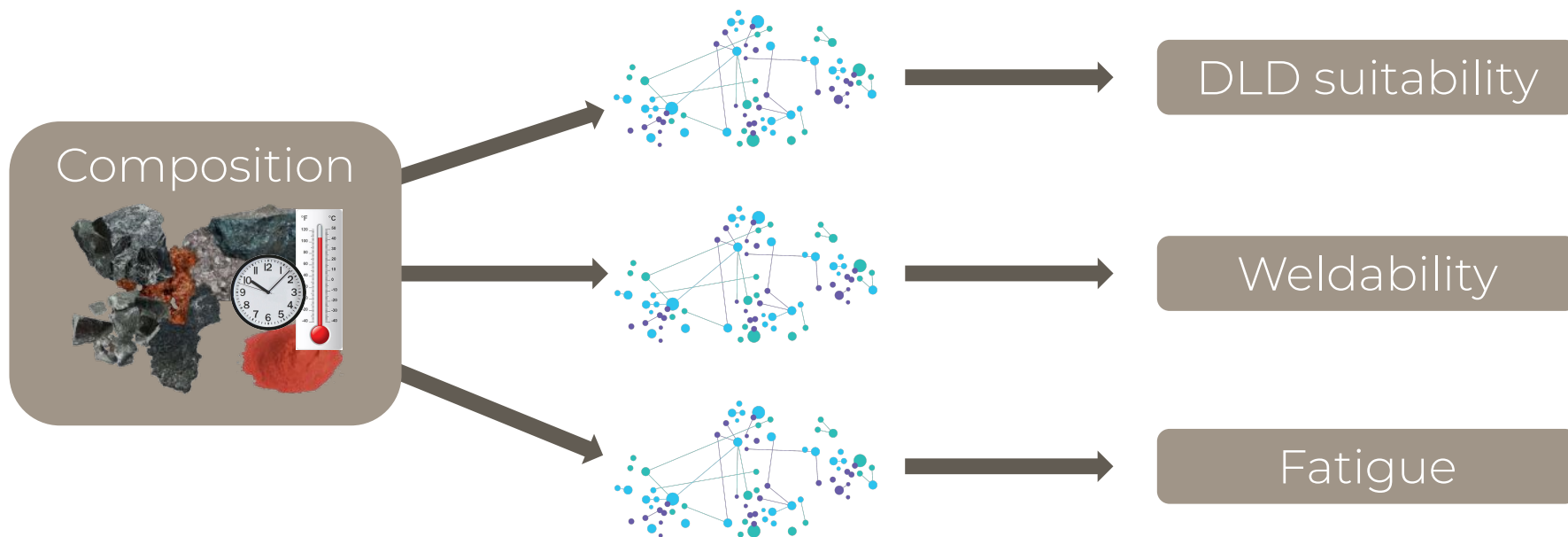
Black box for materials design



Train from existing data



Predict to design new materials



Little data to discover new materials

Only 10 results available for suitability for direct laser deposition

Simplest possible machine learning model is a straight line

$$y = mx + c$$

Little data to discover new materials

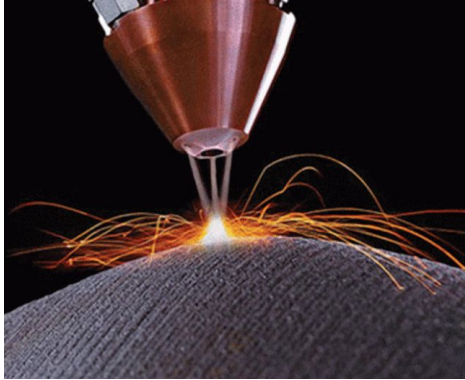
Only 10 results available for suitability for direct laser deposition

Simplest possible machine learning model is a hyperplane

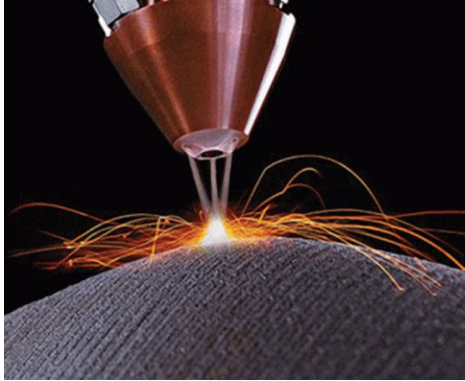
$$y = m_1x_1 + m_2x_2 + m_3x_3 + \dots + m_{30}x_{30} + c$$

Mathematical impossibility to fit 31 variables with 10 pieces of data

Case study: alloy for direct laser deposition



Direct laser deposition is similar to welding

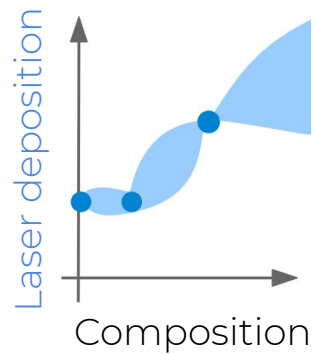


Direct laser
deposition

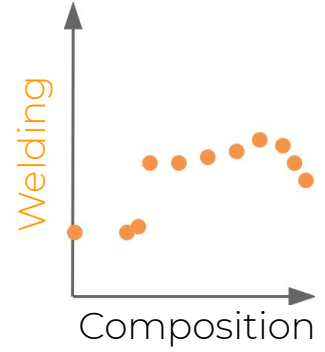
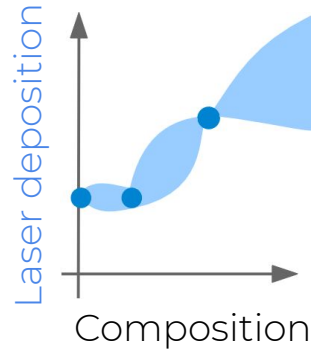


Welding

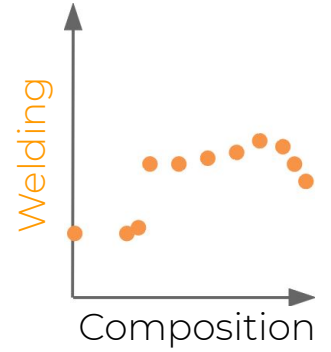
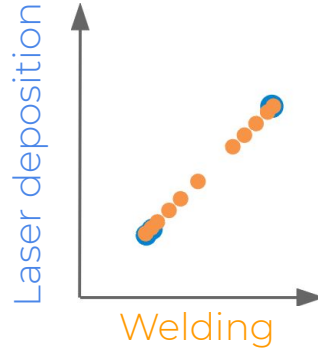
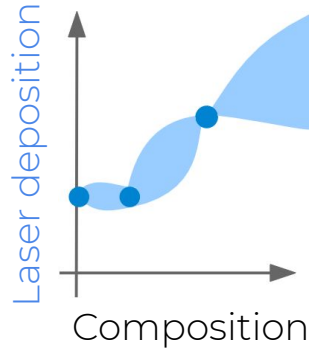
Lack of data for laser deposition



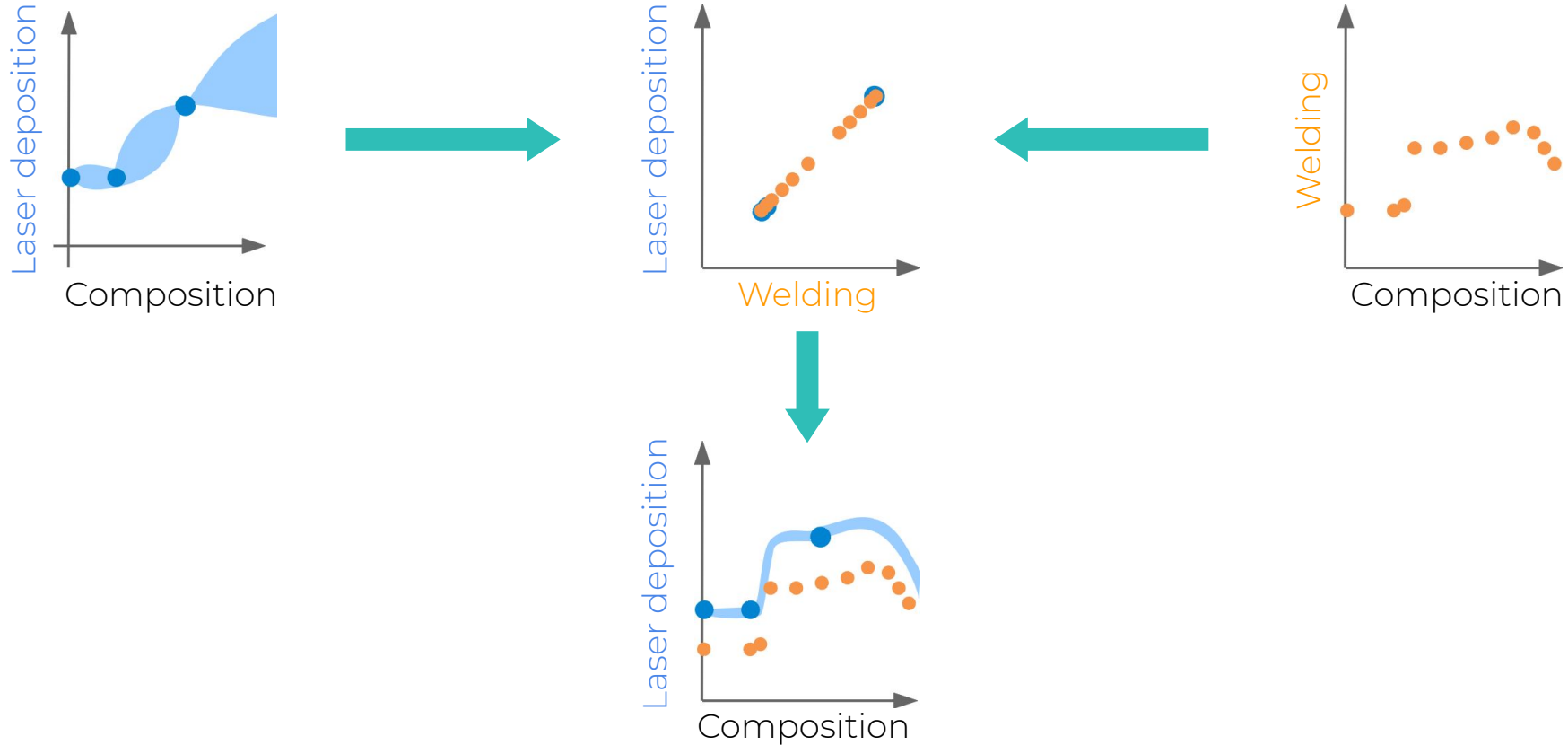
Large amount of welding data



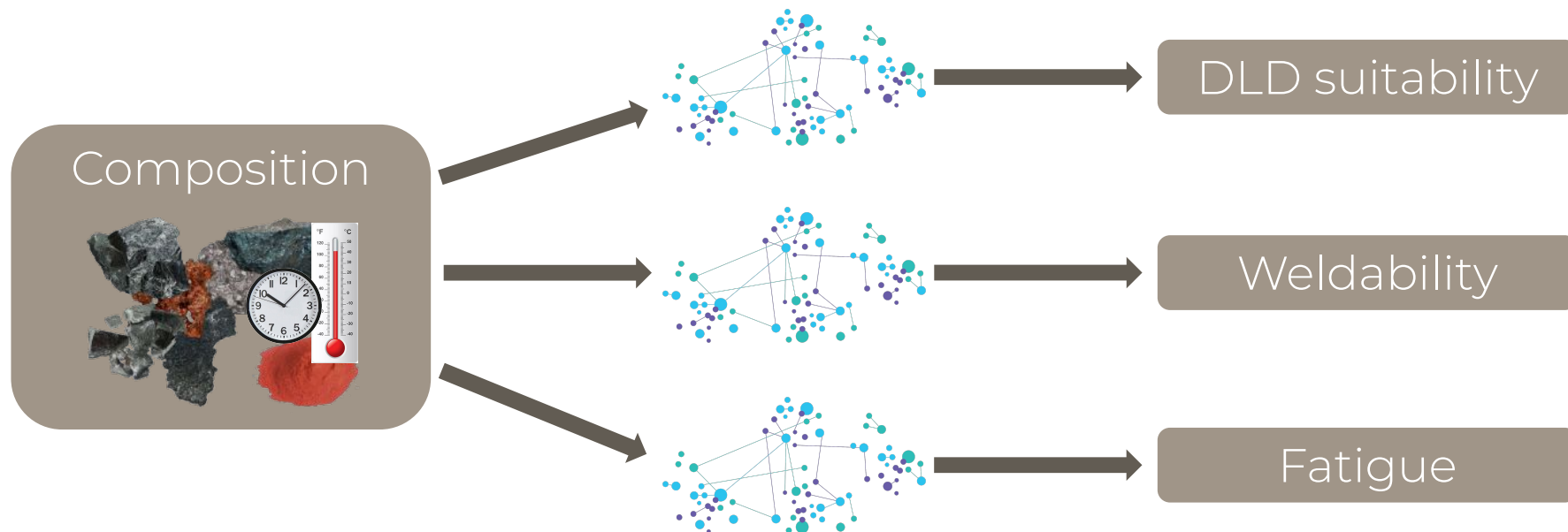
Simple welding-deposition relationship



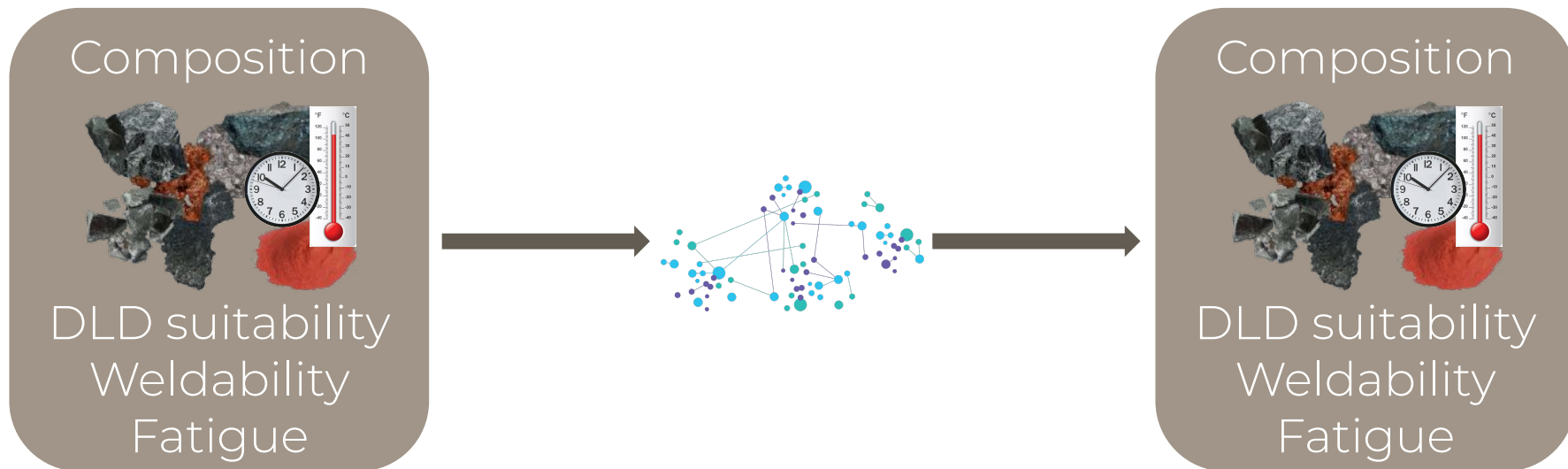
Welding data guides extrapolation



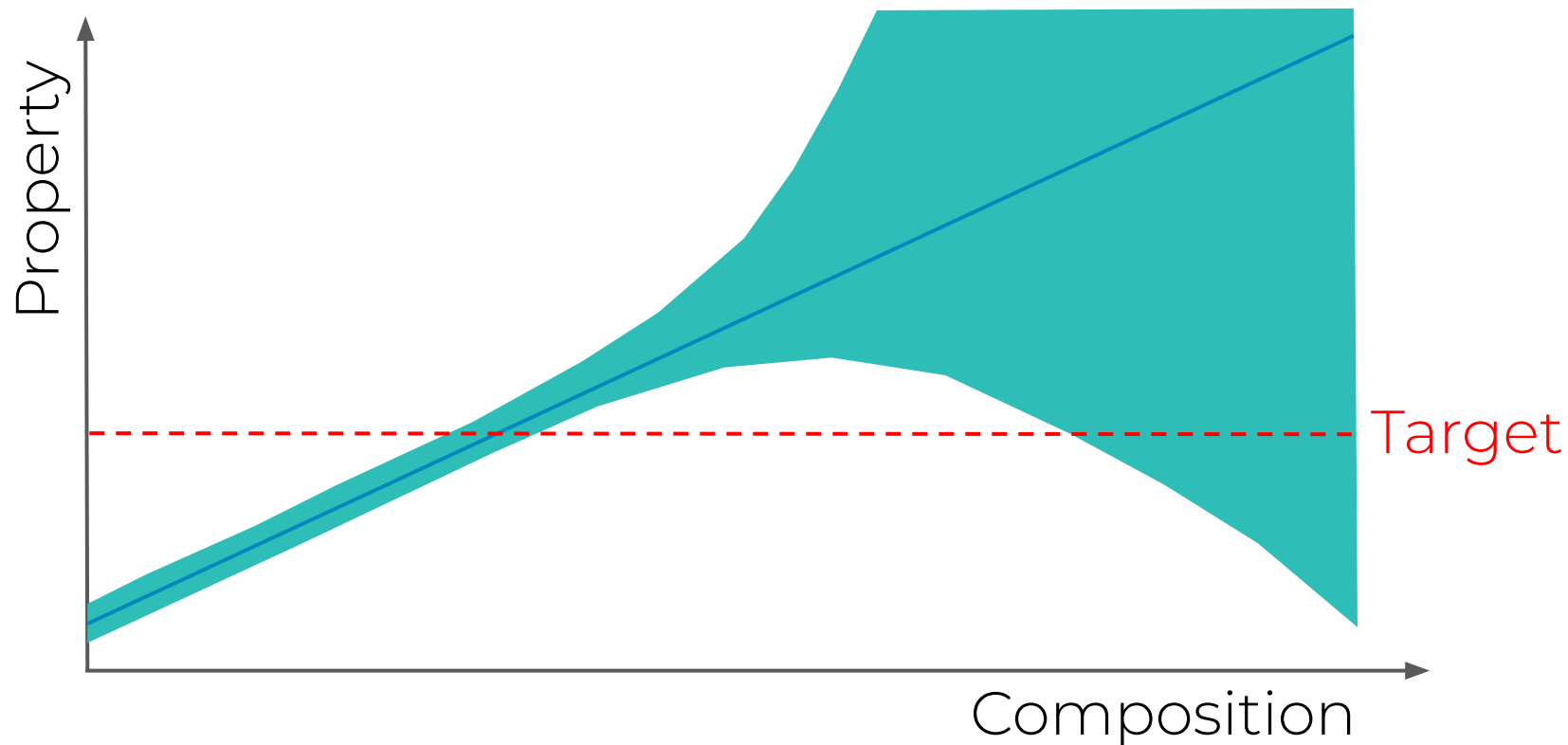
Standard machine learning



Holistic machine learning for materials design



Maximize likelihood of alloy exceeding targets



Targets for direct laser deposition alloy

Elemental cost	< 25 \$kg ⁻¹
Density	< 8500 kgm ⁻³
γ' content	< 25 wt%
Oxidation resistance	< 0.3 mgcm ⁻²
DLD suitability	< 0.15% defects
Phase stability	> 99.0 wt%
γ' solvus	> 1000 °C
Thermal resistance	> 0.04 K Ω ⁻¹ m ⁻³
Yield stress at 900 °C	> 200 MPa
Tensile strength at 900 °C	> 300 MPa
Tensile elongation at 700 °C	> 8%
1000hr stress rupture at 800 °C	> 100 MPa
Fatigue life at 500 MPa, 700 °C	> 10 ⁵ cycles

Composition of alloy for direct laser deposition

Cr 19%



Co 4%



Mo 4.9%



W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



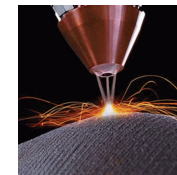
B 0.01%



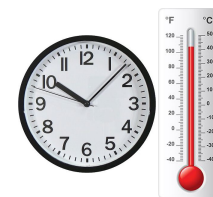
Ni balance



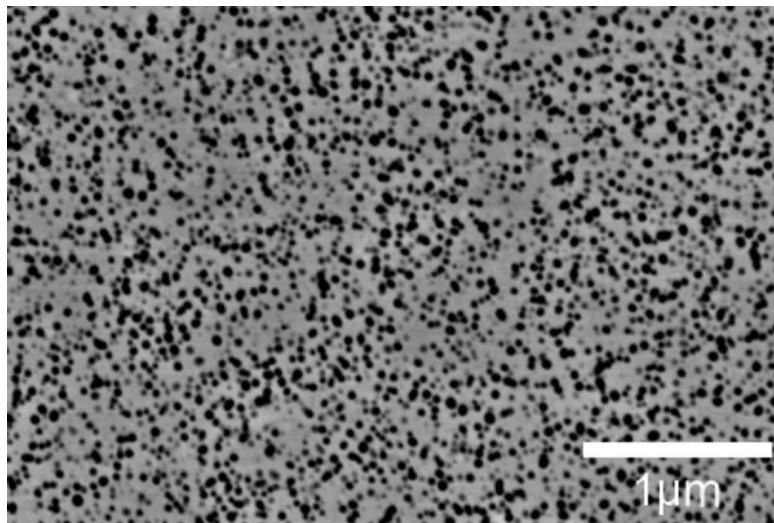
Expose 0.8



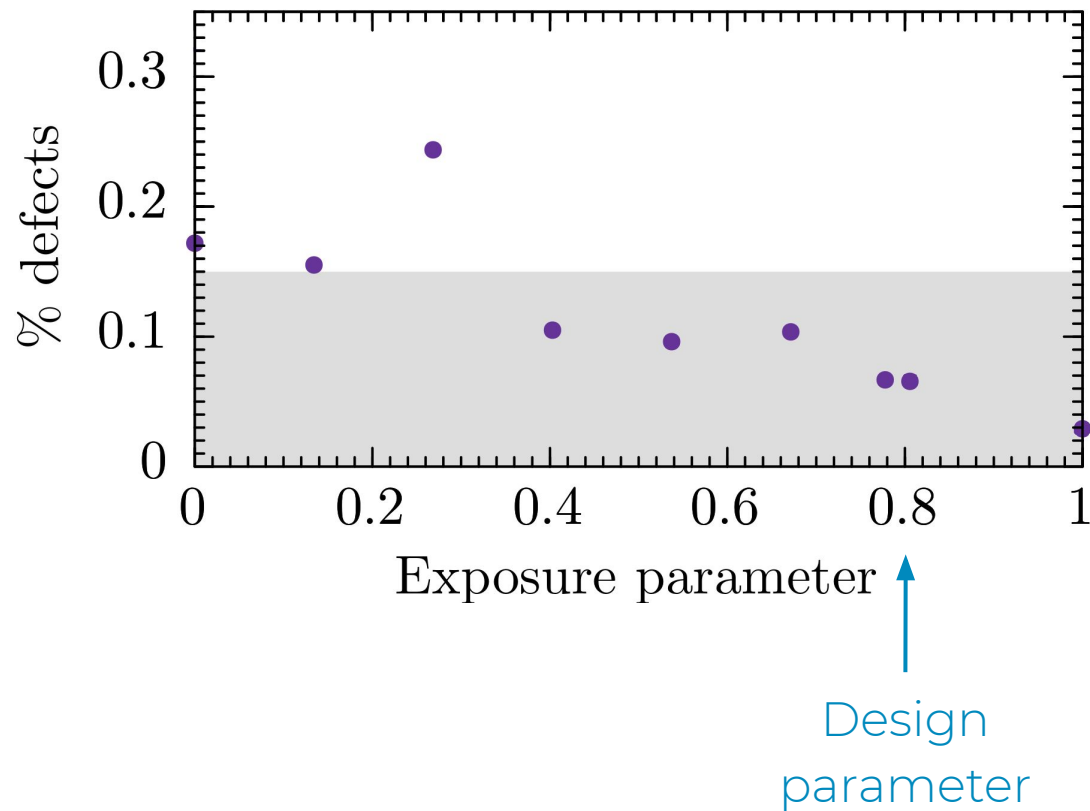
T_{HT} 1230°C



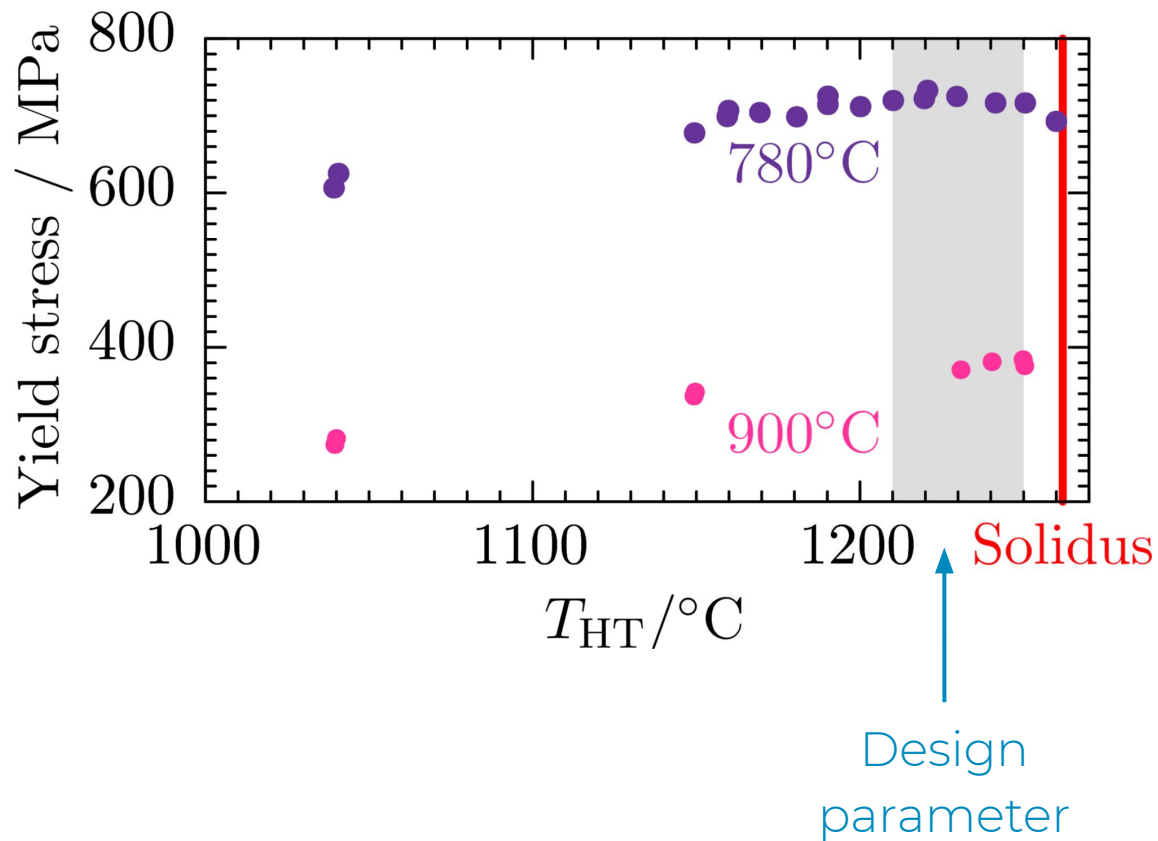
Experimental validation: microscope



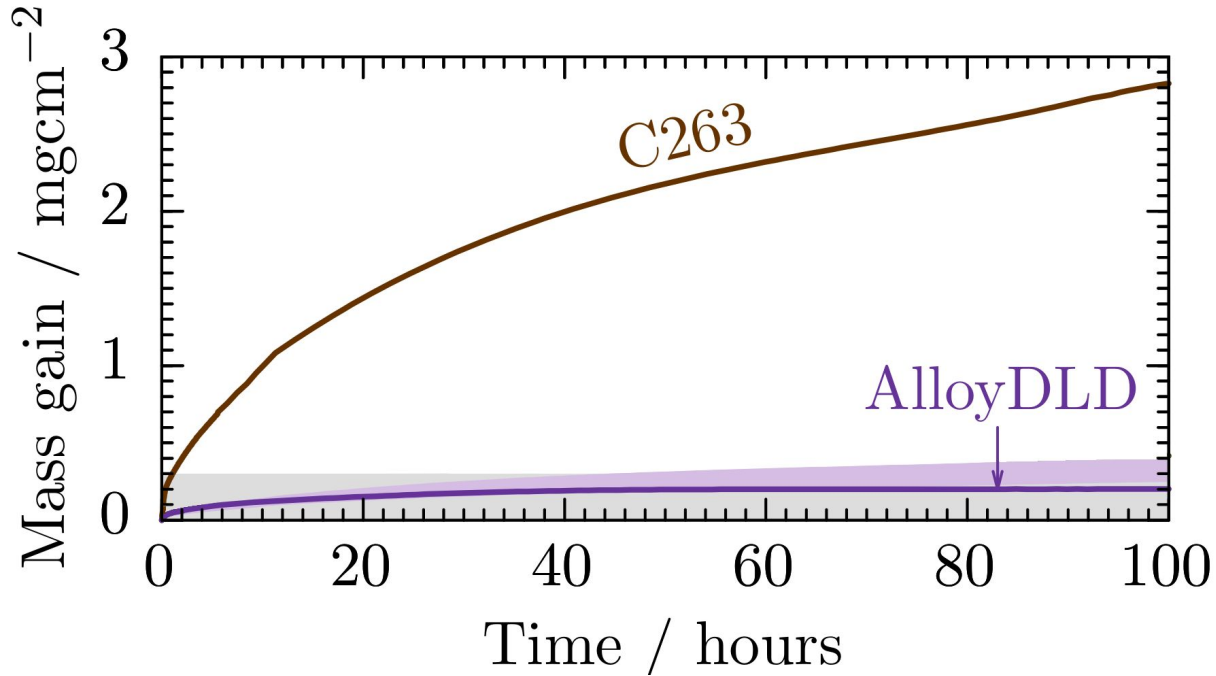
Experimental validation: defects



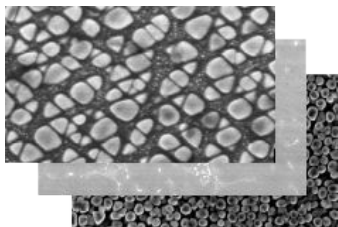
Experimental validation: yield stress



Experimental validation: oxidation resistance



Further materials design



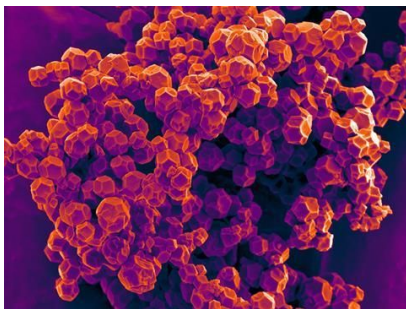
Nickel & moly alloys



Batteries



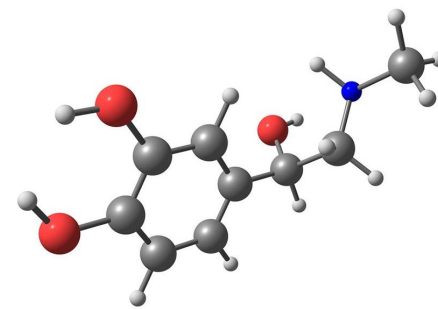
Steels of welding



Metal-organic framework

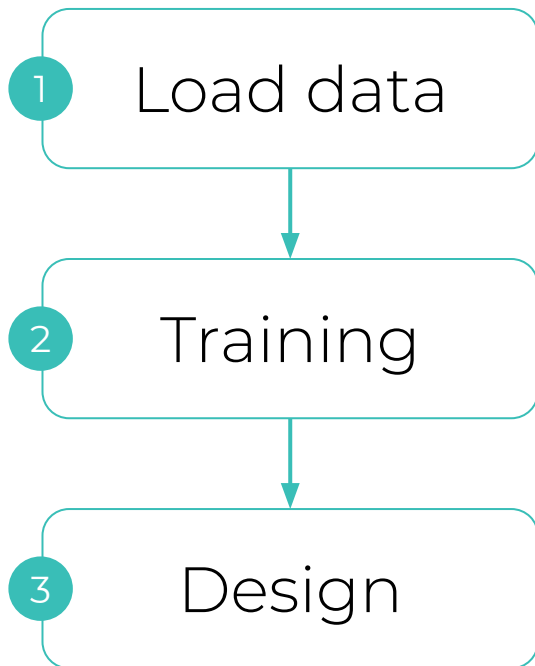


Concrete



Pharmaceutical

Future opportunities: Integrated software



Predicting properties of steel

We demonstrate a neural network that predicts the physical properties of steels based on the composition and heat treatment. The neural network model was trained from a library of experimental data from 1000 alloys.


In the first panel below set the percentages of each element in the composition and heat treatment temperature, and then click predict to get the neural network estimates for yield stress, ultimate tensile strength, and elongation.

Click [here](#) to use this technology to optimize the yield stress, ultimate tensile strength, and elongation the steel.

This same technology was used to understand nickel alloys where the composition covered 20 elements, 5 heat treatment parameters, and predicted 11 material properties. Click here to read more about this study.

Click here to optimize a composition for given targets

Set inputs		
Iron (Fe)	<input type="text" value="100"/>	remain %
Carbon (C)	<input type="text" value="0"/>	0 to 0.43 %
Manganese (Mn)	<input type="text" value="0"/>	0 to 3.0 %
Silicon (Si)	<input type="text" value="0"/>	0 to 4.75 %
Chromium (Cr)	<input type="text" value="0"/>	0 to 17.5 %
Nickel (Ni)	<input type="text" value="0"/>	0 to 21.0 %
Molybdenum (Mo)	<input type="text" value="0"/>	0 to 9.67 %
Vanadium (V)	<input type="text" value="0"/>	0 to 4.32 %

 PREDICT

Predictions	
Yield Stress (MPa)	1605 ± 46
Ultimate Tensile Strength (MPa)	1200 ± 67
Elongation (%)	9 ± 2

Design and interrogate new materials

Alchemite Prepared models Materials design company: Material

MATERIAL for Model for hardness_loss_v2.csv: 574 (2038)

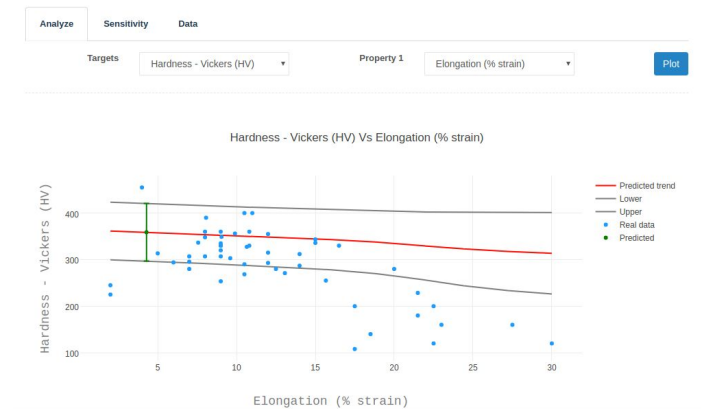
Data Analyze Design Materials Home

Design Material

Please use the form below to add desired targets variables, other variables will be optimised

Design globally or locally

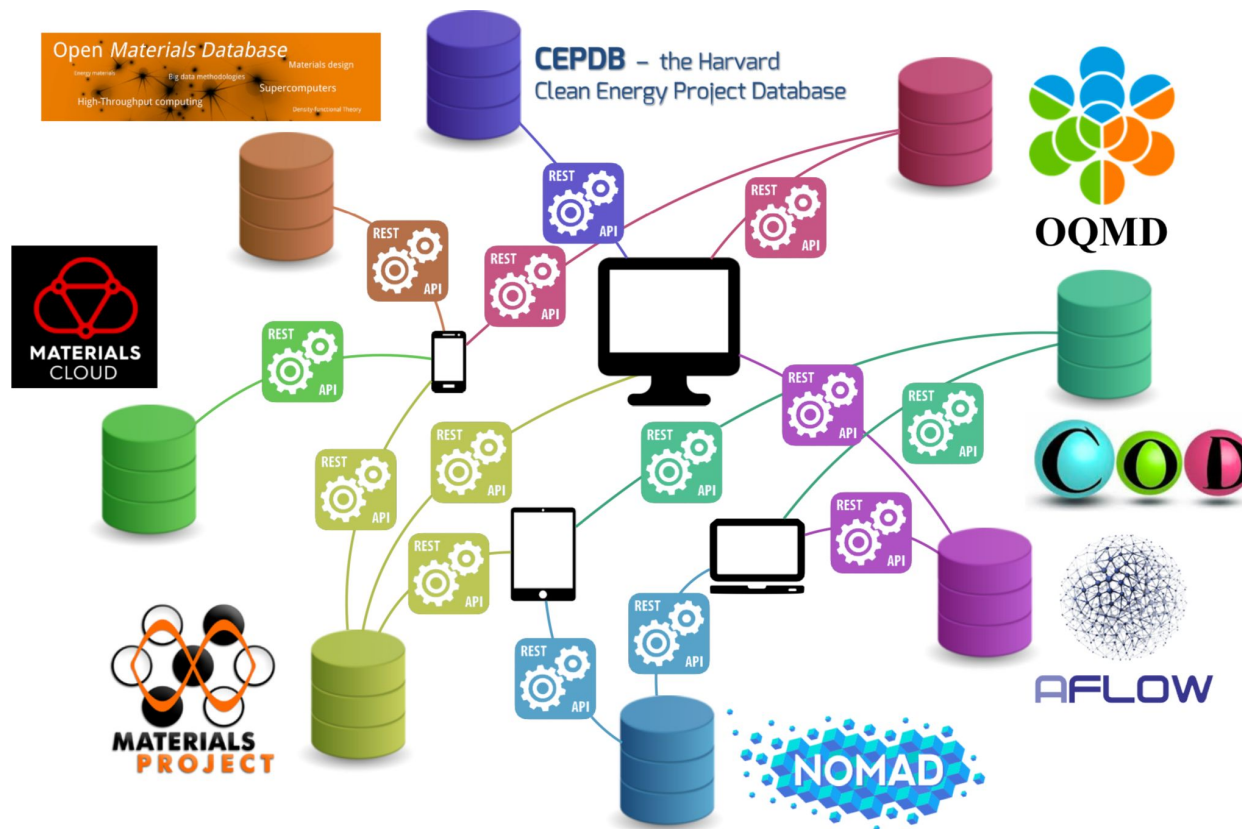
Type	Name	Value	Target	Designed values	Uncertainty
	C (0.0 - 5.91)	<input type="text" value="0.035"/>	Target: Above		
	Mn (0.0 - 15.58)	<input type="text" value="0.88"/>	Target: Exact		
	Si (0.0 - 2.07)	<input type="text" value="0.43"/>	Design start		
	Cr (0.0 - 32.6)	<input type="text" value="1.6"/>	Design start		
	Mo (0.0 - 6.3)	<input type="text" value="0.37"/>	Design start		
	V (0.0 - 1.25)	<input type="text" value="0.0"/>	Design start		
	Nb (0.0 - 6.46)	<input type="text" value="0.0"/>	Design start		



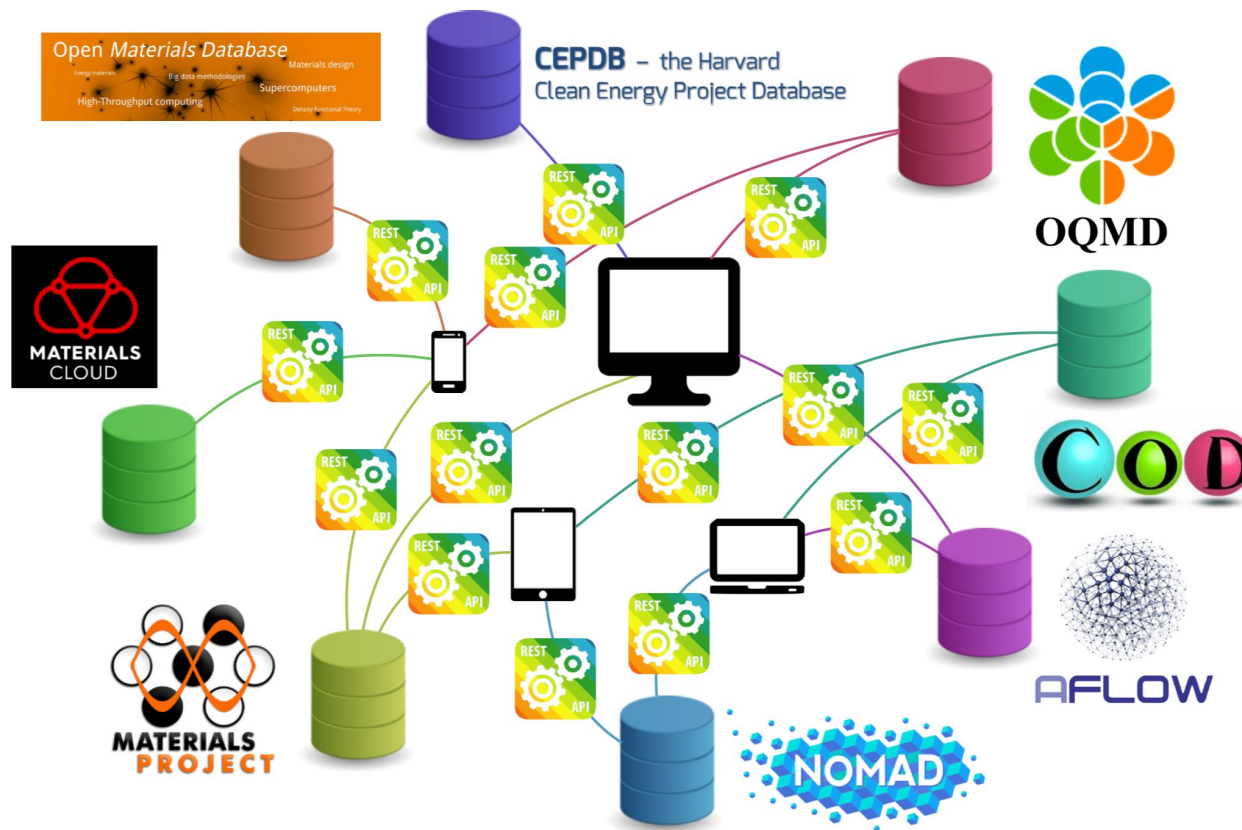
Zoo of materials databases



Labor intensive to harvest data



Universal API would ease access





A **RESTful API** to access leading electronic structure materials databases

Supported by CECAM to now extend to **molecular dynamics** and bio-simulations

<http://www.optimade.org/>

Machine learning for materials design

Merge sparse databases to deliver deep insights into new materials

Designed and **experimentally verified** alloy for direct laser deposition, and other alloys and drugs

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Demo	https://app.intellegens.ai/steel_optimise
Papers	https://www.intellegens.ai/paper.html