Intellegens

UNIVERSITY OF CAMBRIDGE

The modern-day blacksmith

Gareth Conduit

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

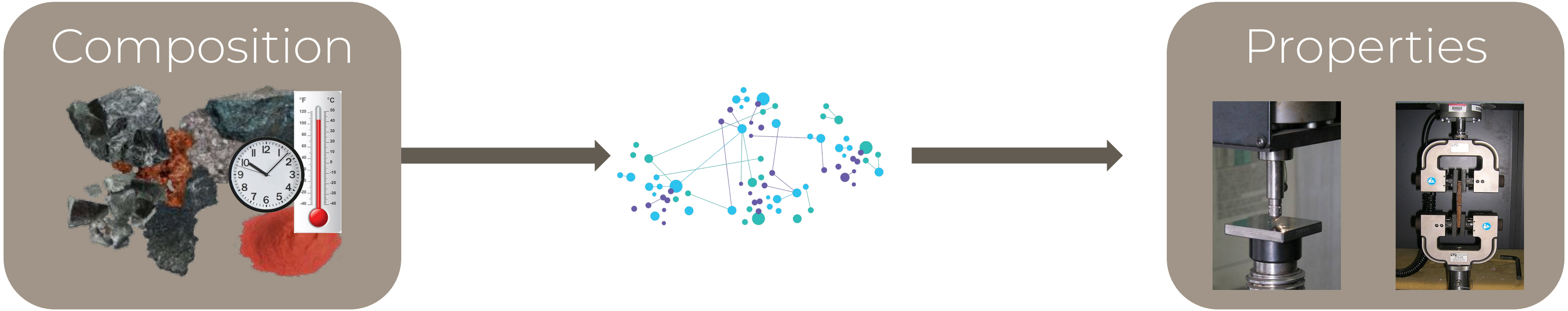
Traditional experimental design

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

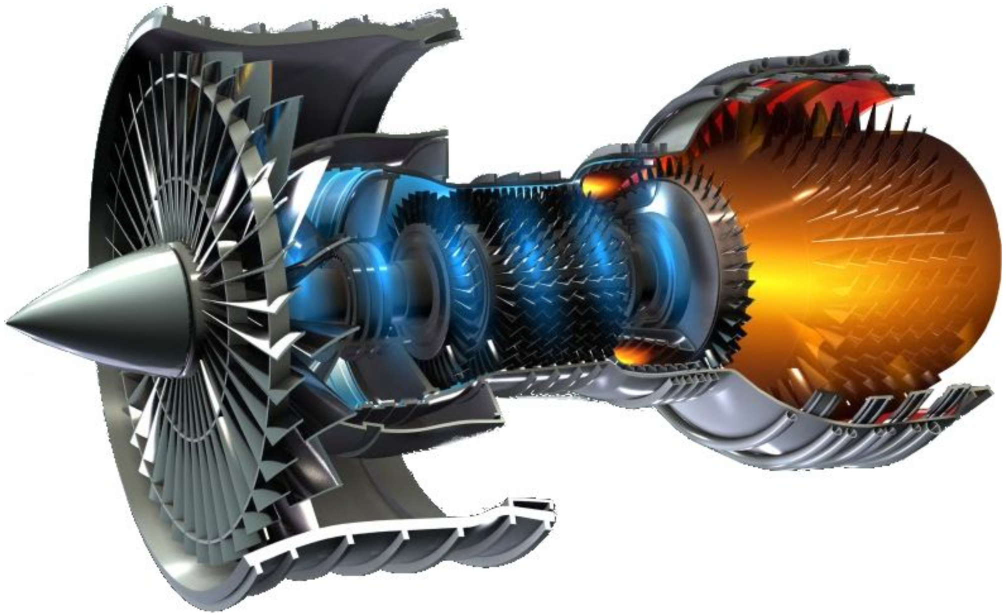
Typical experimental data is 0.2% complete so algorithm must handle missing data

Optimized design process

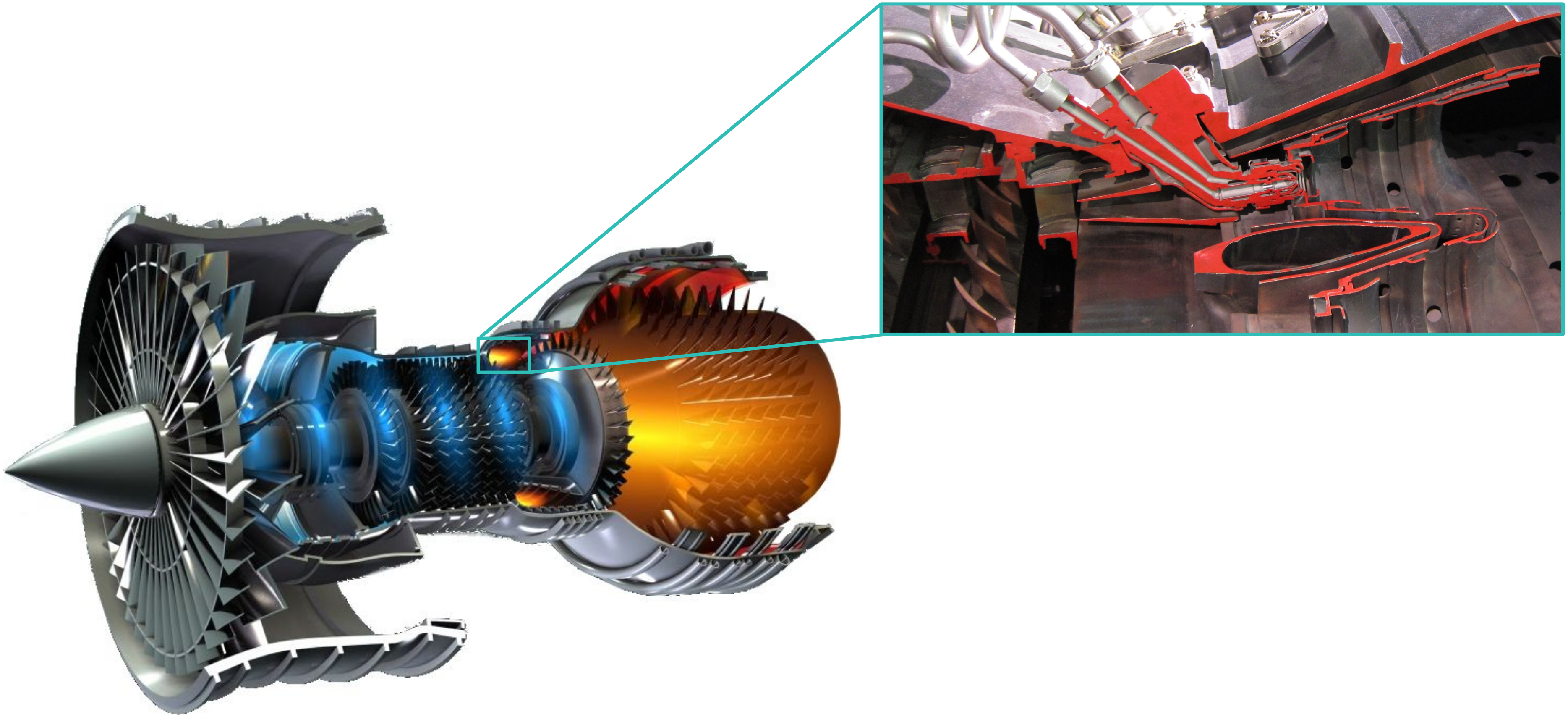
Reduce costs - 90% reduction in experiments and fewer measurements for expensive quantities

Accelerate discovery and validation to 2 years

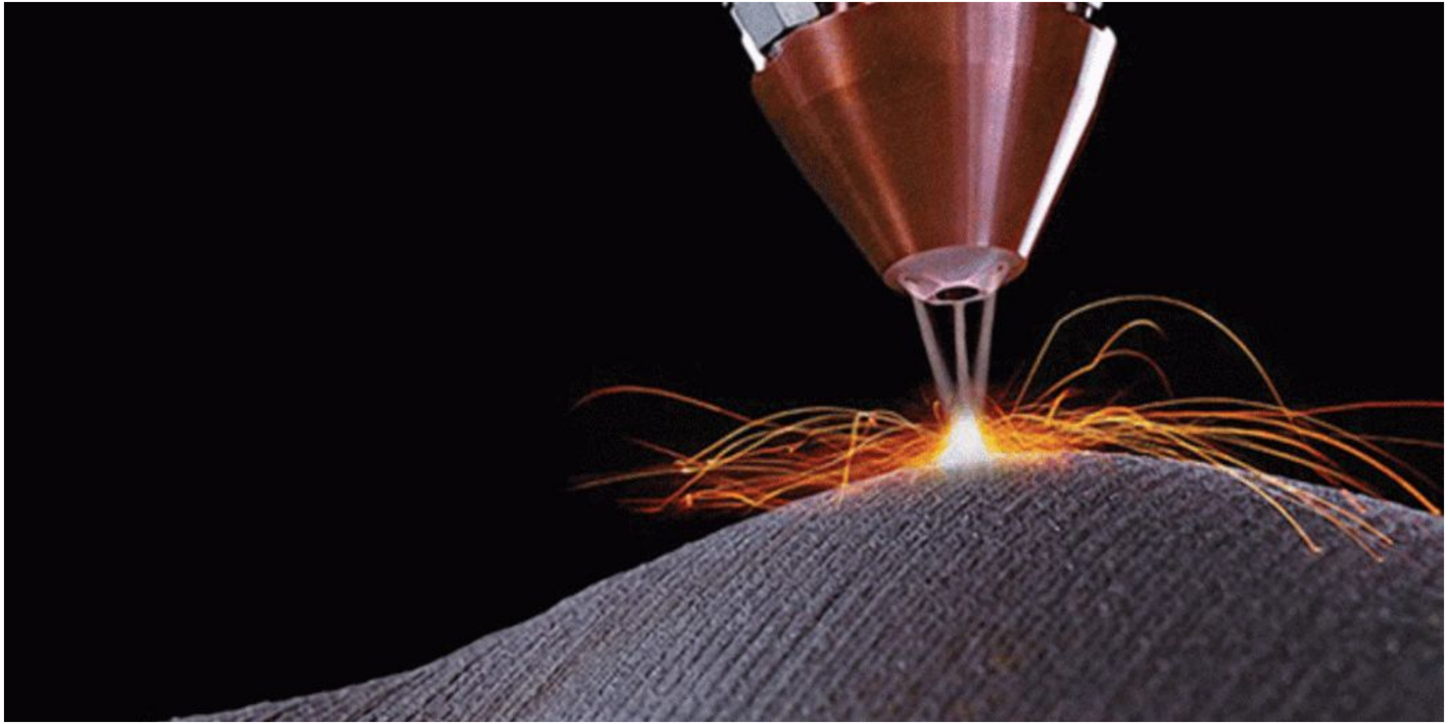
Schematic of a jet engine



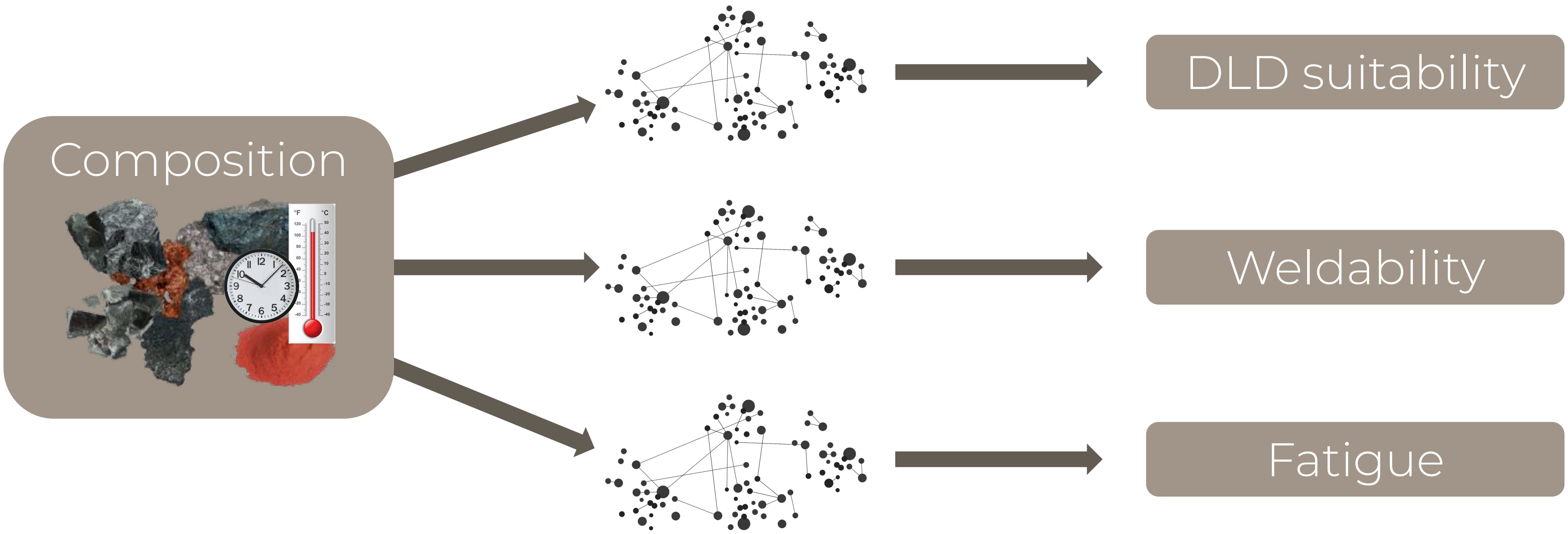
Combustor in a jet engine



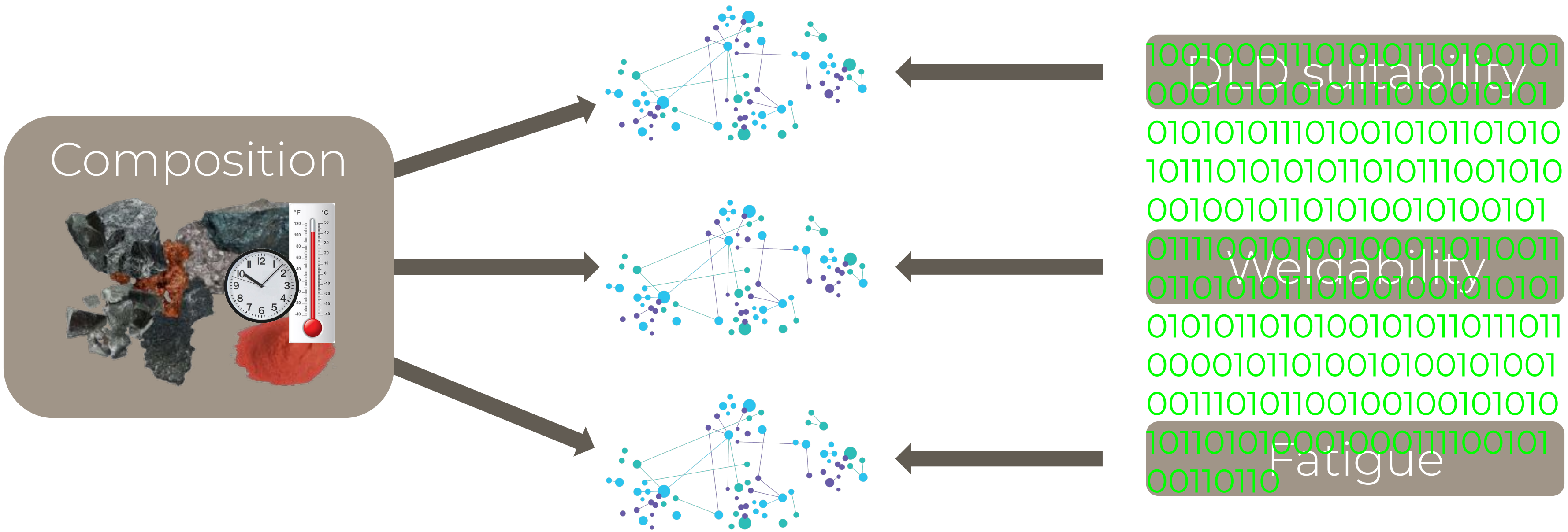
Direct laser deposition requires new alloys



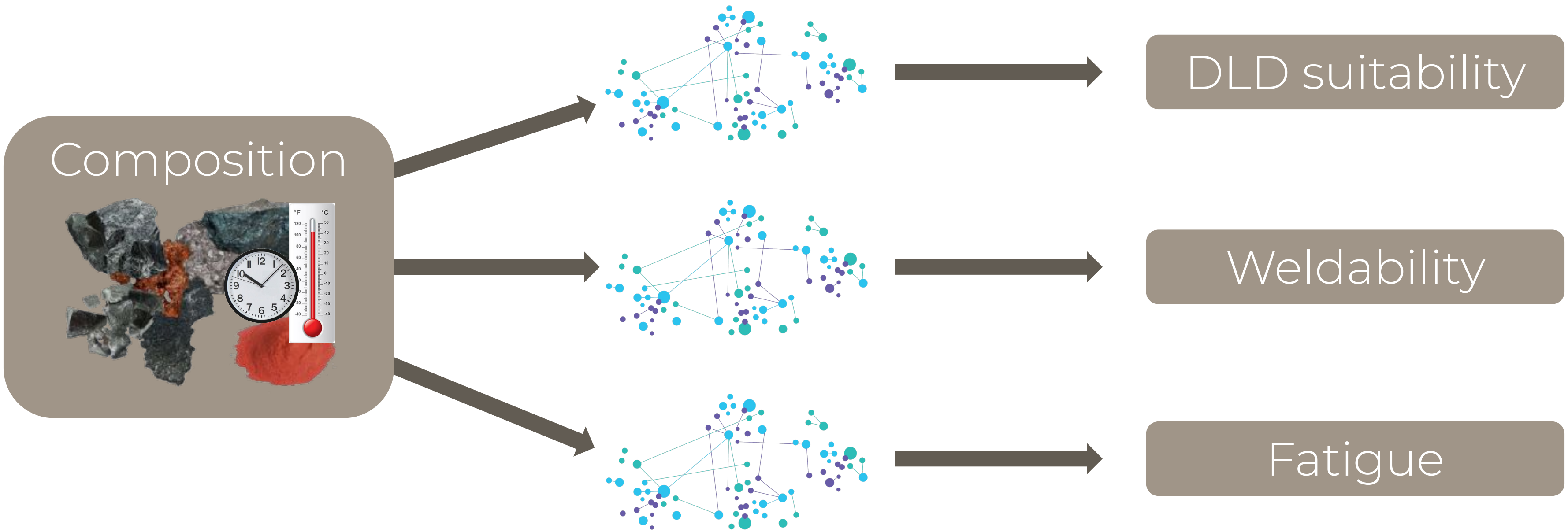
Black box for materials design



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

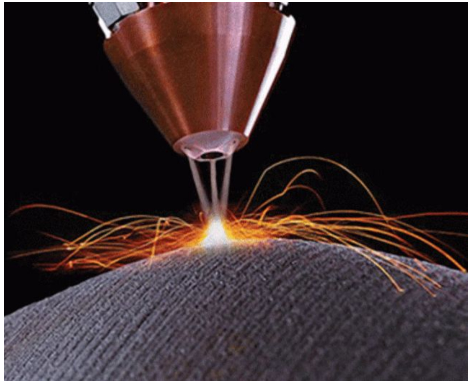
Only 10 results available for suitability for direct laser deposition

Simplest possible machine learning model is a hyperplane

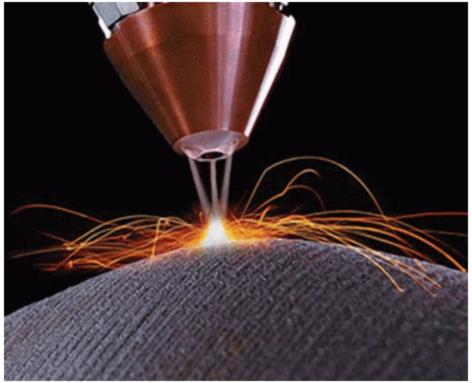
$$y = m_1x_1 + m_2x_2 + m_3x_3 + \ldots + m_{30}x_{30} + c$$

Mathematical impossibility to fit 31 variables with 10 pieces of data

Case study: alloy for direct laser deposition



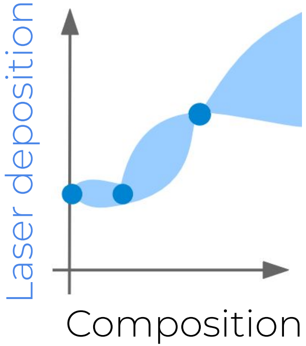
Direct laser deposition is similar to welding



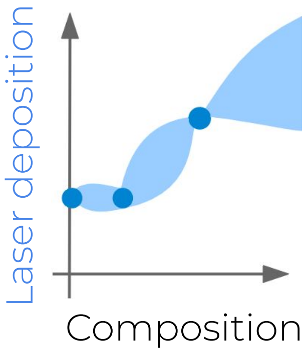
Direct laser deposition

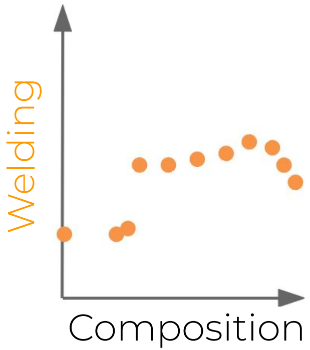
Welding

Lack of data for laser deposition

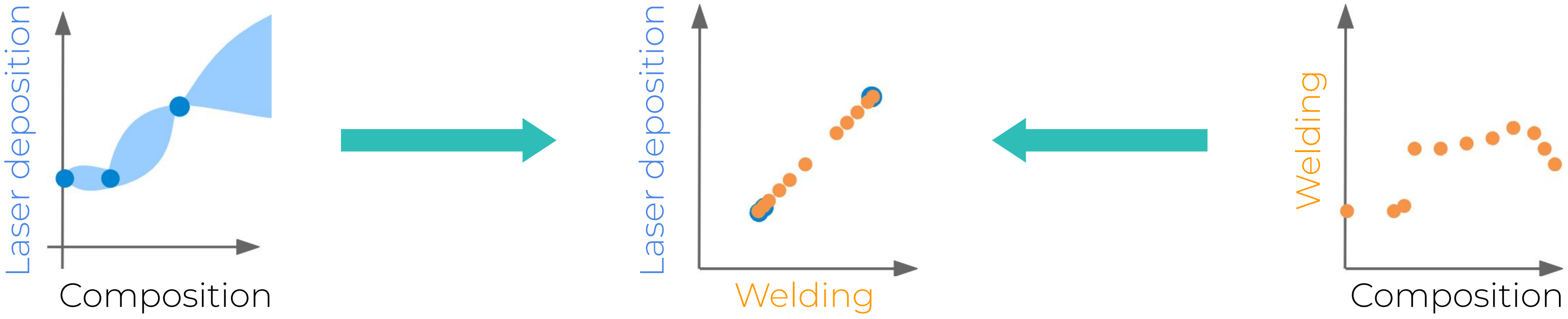


Large amount of welding data





Simple welding-deposition relationship



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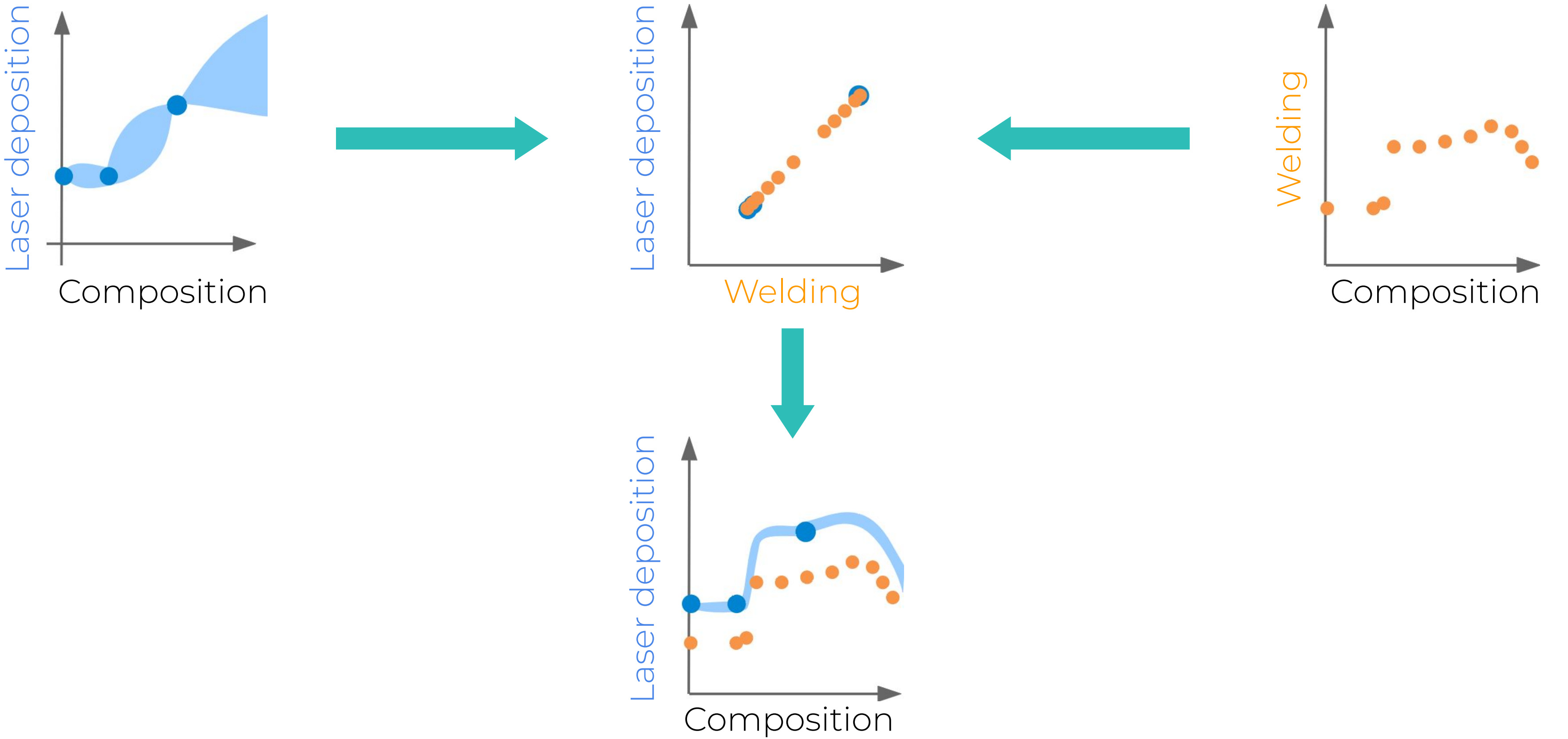
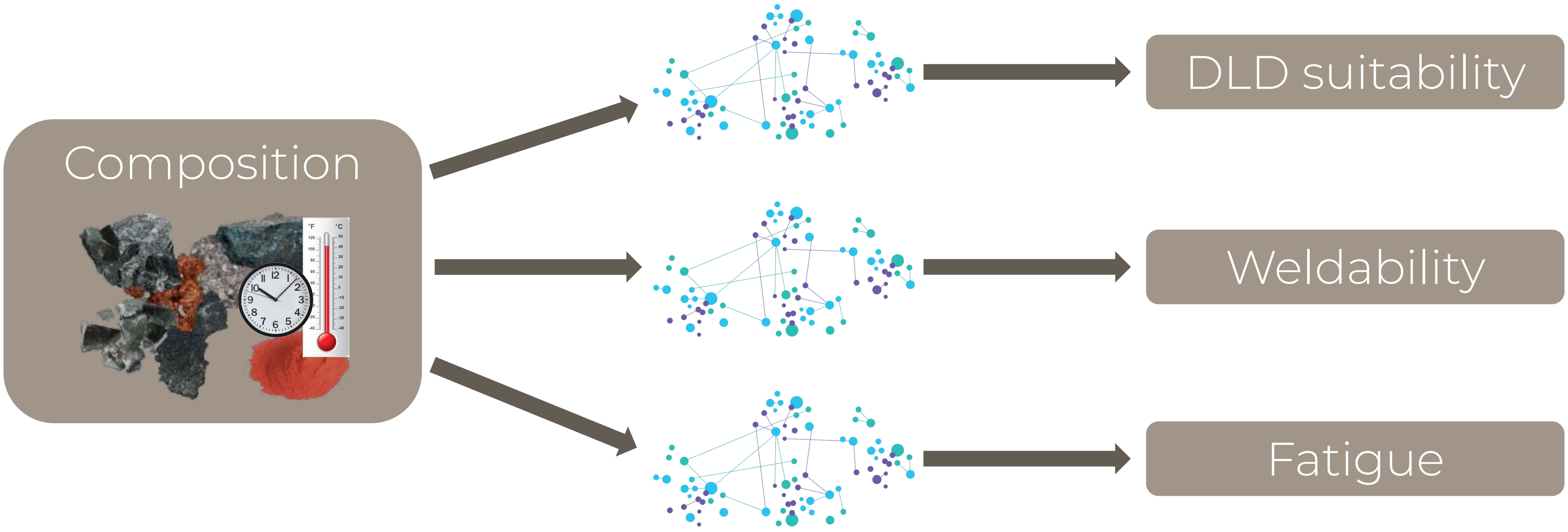
Welding data guides extrapolation

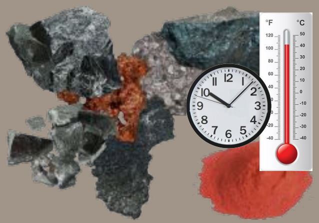


Standard machine learning



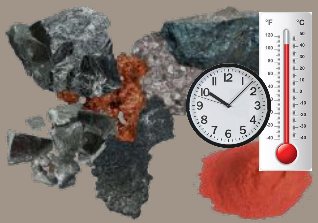
Holistic machine learning for materials design

Composition



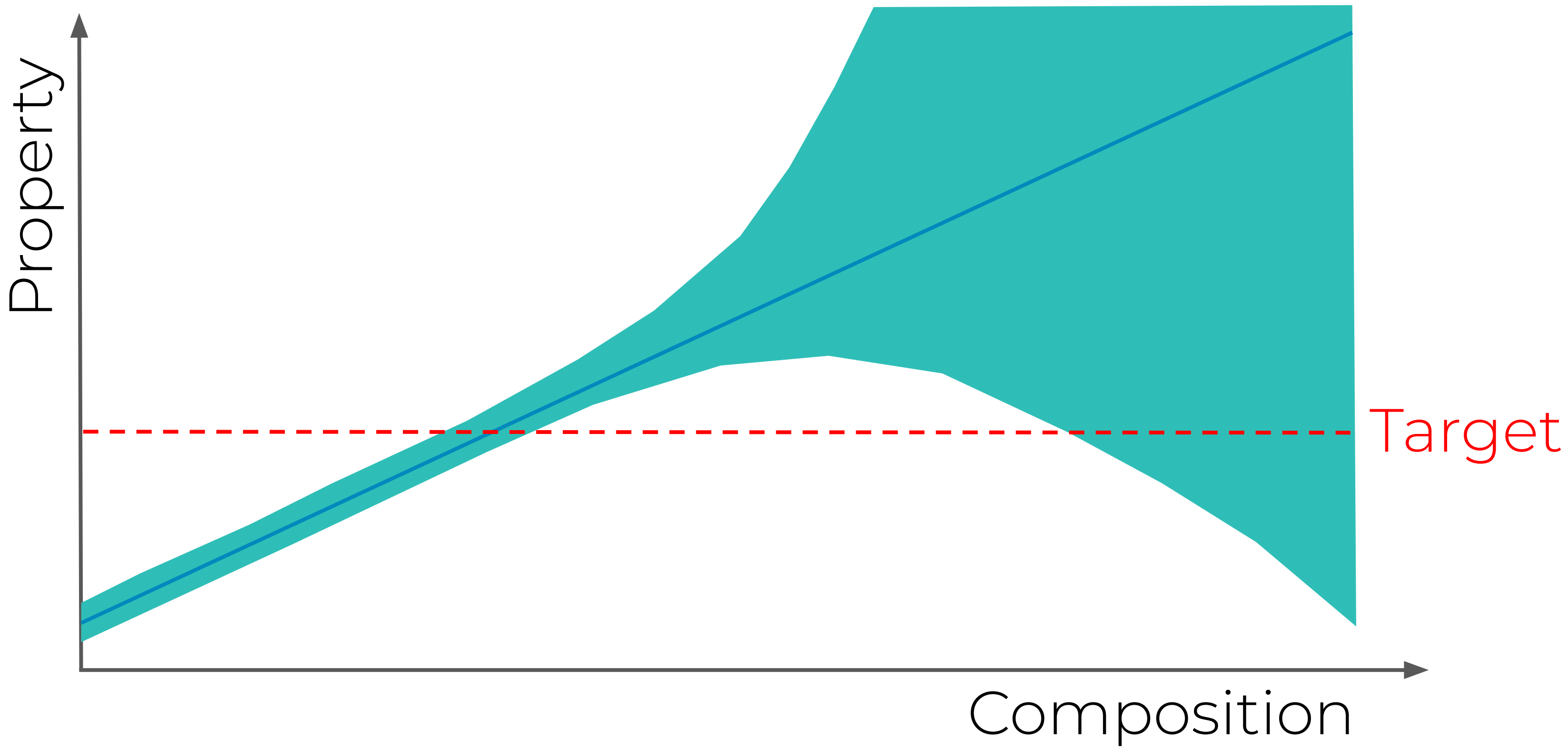
DLD suitability
Weldability
Fatigue

Composition



DLD suitability
Weldability
Fatigue

Maximize likelihood of alloy exceeding targets



Targets for direct laser deposition alloy

Elemental cost	$< 25\ \$\mathrm{kg}^{-1}$
Density	$< 8500\ \mathrm{kgm}^{-3}$
γ’ content	< 25 wt%
Oxidation resistance	$< 0.3\ \mathrm{mgcm}^{-2}$
DLD suitability	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	$> 0.04\ \mathrm{K}\Omega^{-1}\mathrm{m}^{-3}$
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%

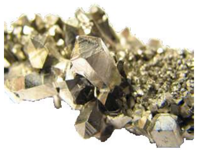
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



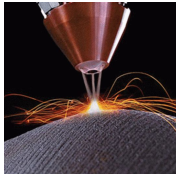
Al 2.9%

C 0.04%

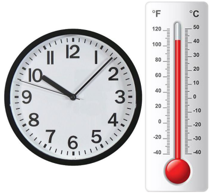
B 0.01%

Ni balance

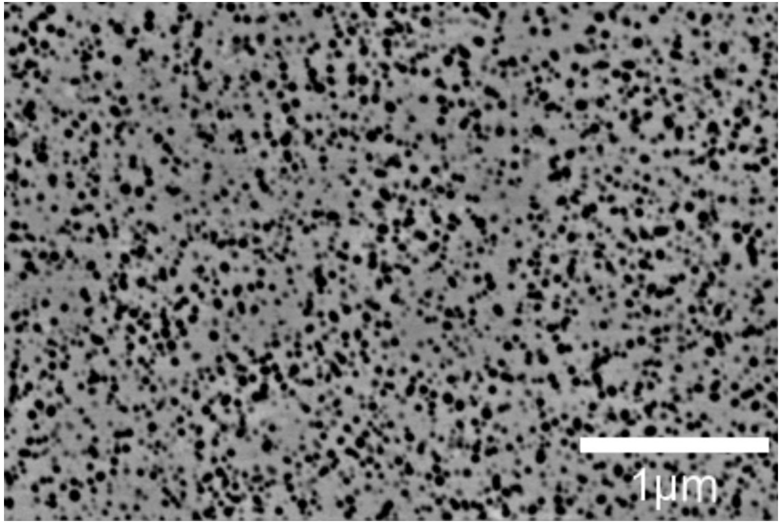
Expose 0.8



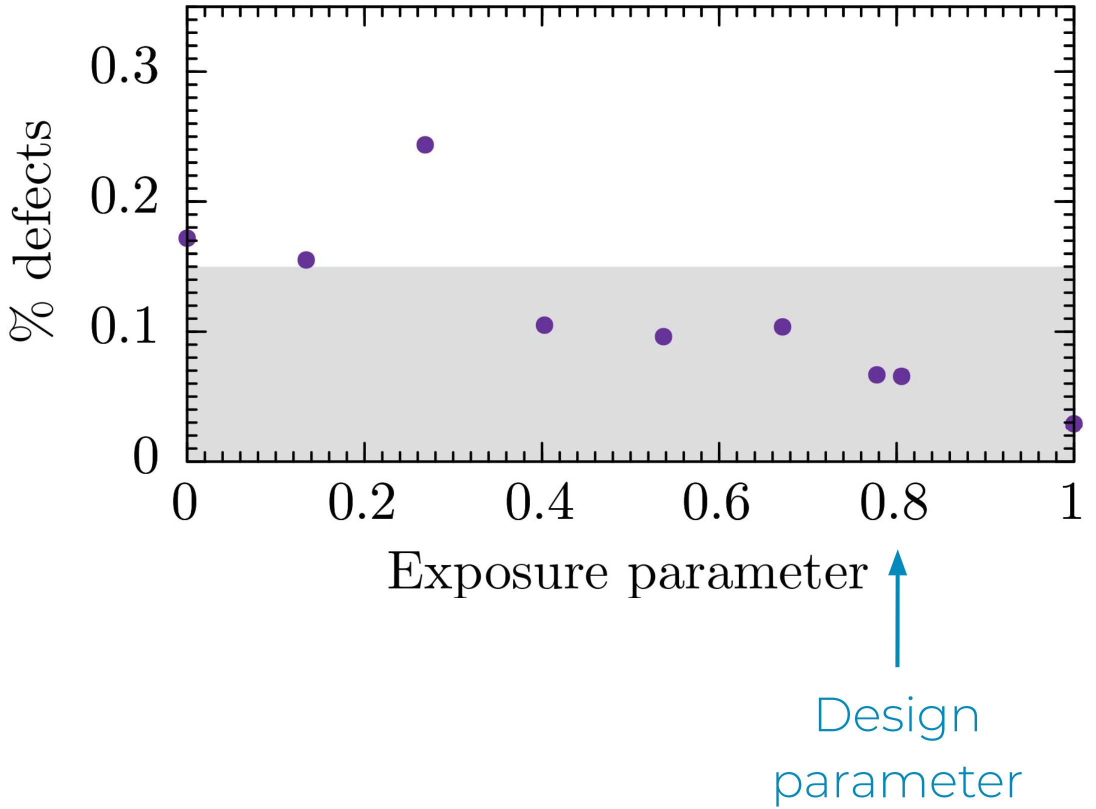
T_{HT} 1230°C



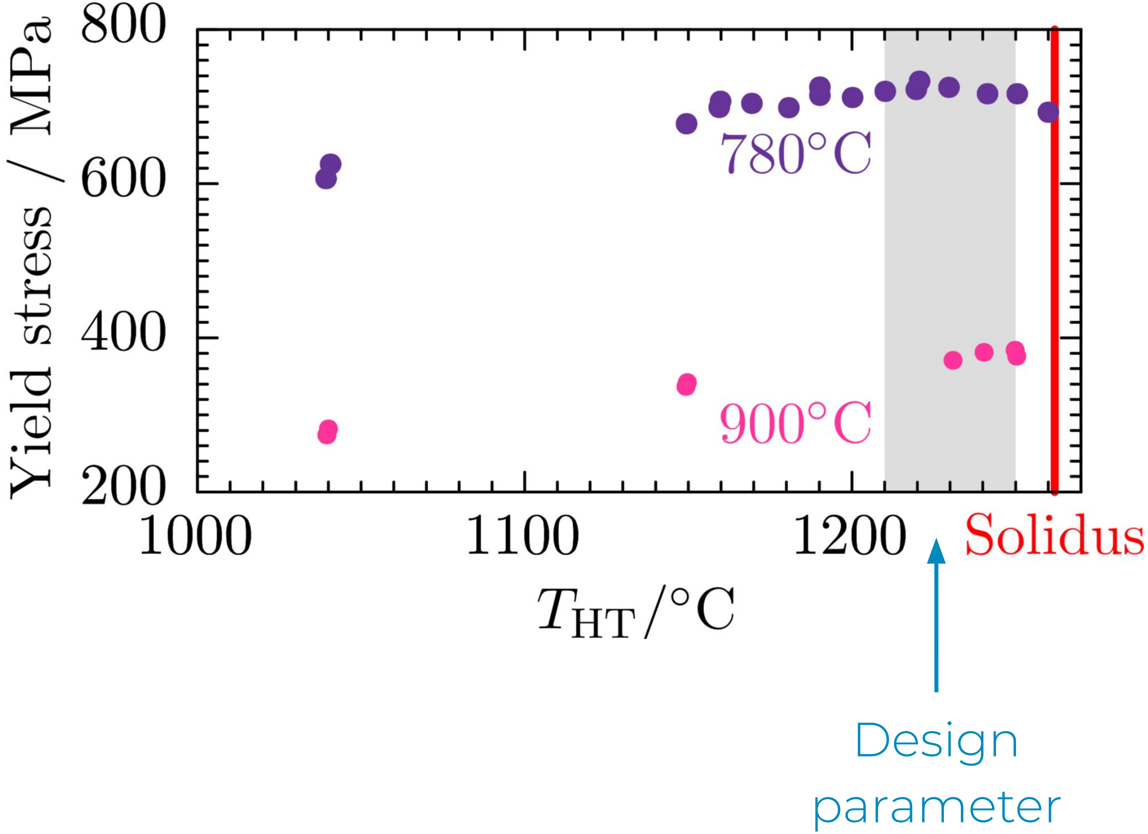
Experimental validation: microscope



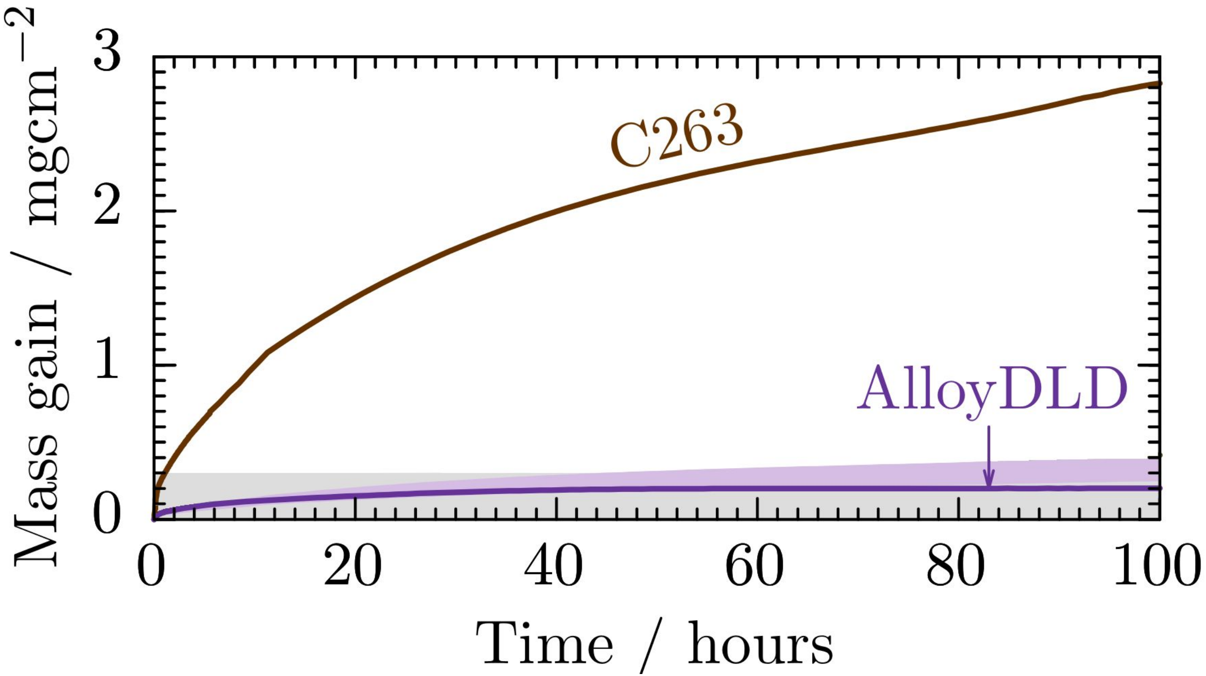
Experimental validation: defects



Experimental validation: yield stress



Experimental validation: oxidation resistance



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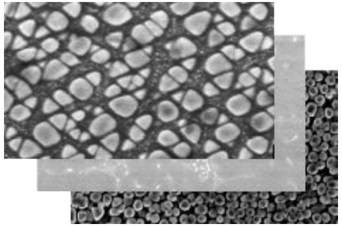
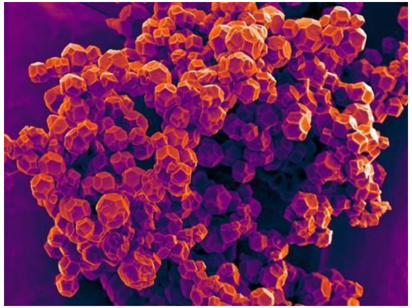
Further materials design



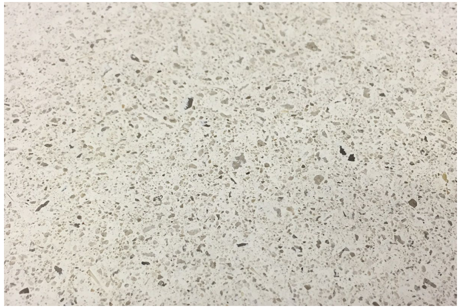
Nickel & moly alloys

Batteries

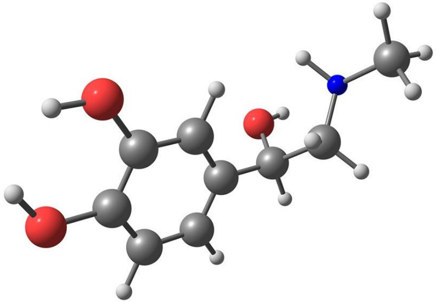
Steels of welding



Metal-organic framework



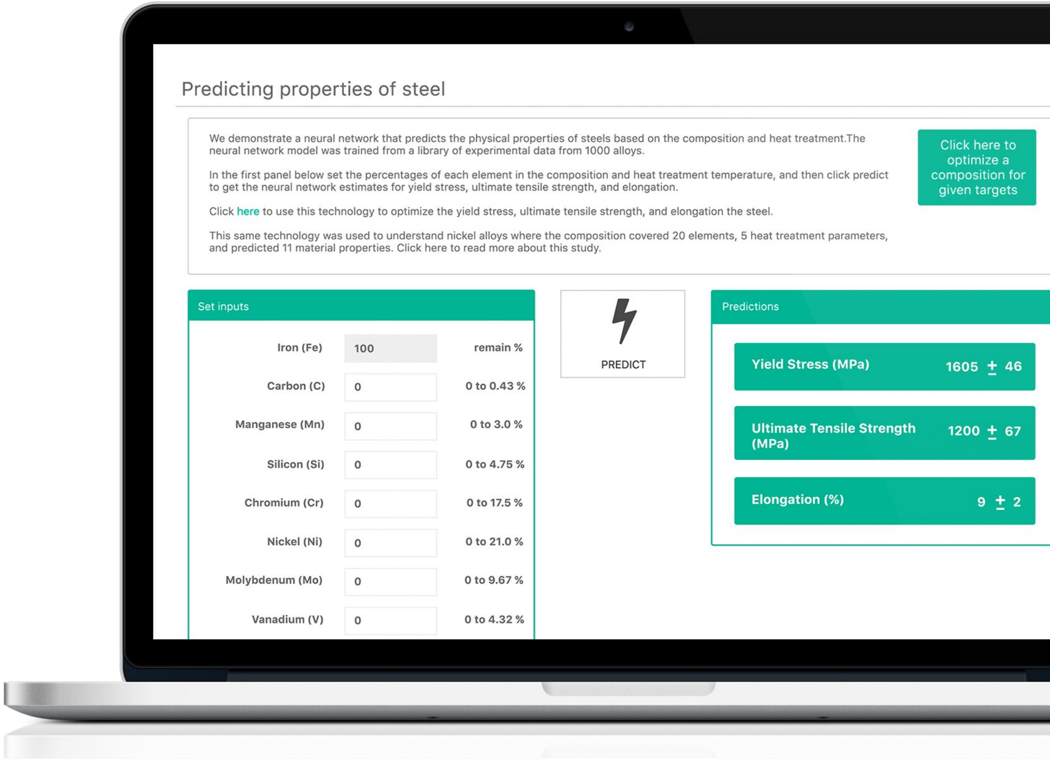
Concrete



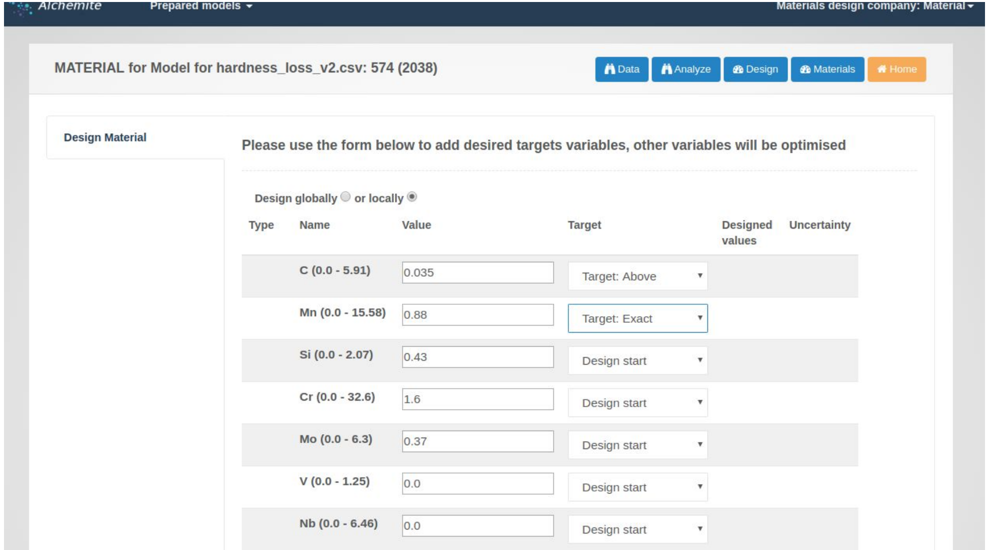
Pharmaceutical

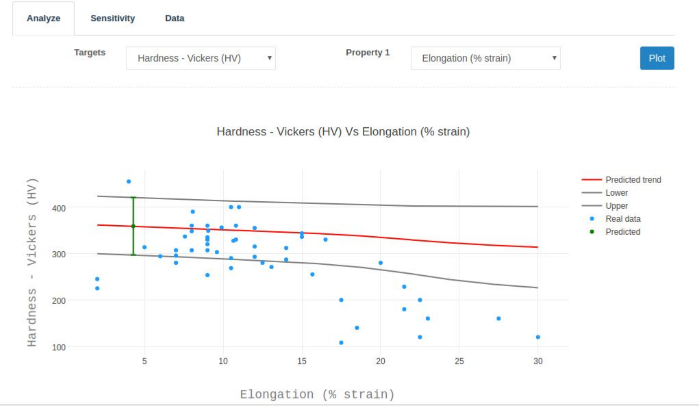
Future opportunities: Integrated software

1. Load data
2. Training
3. Design

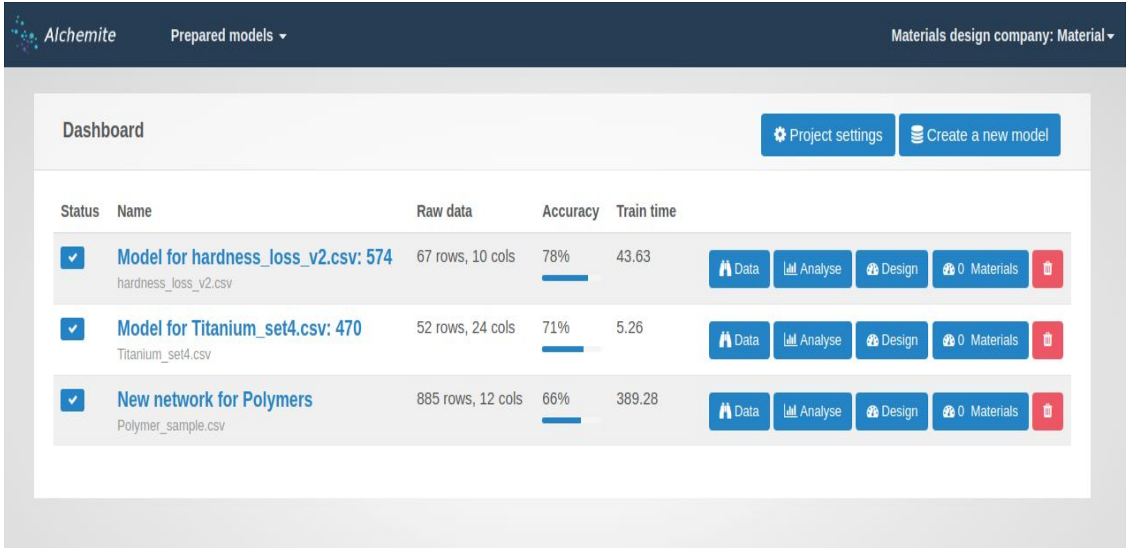


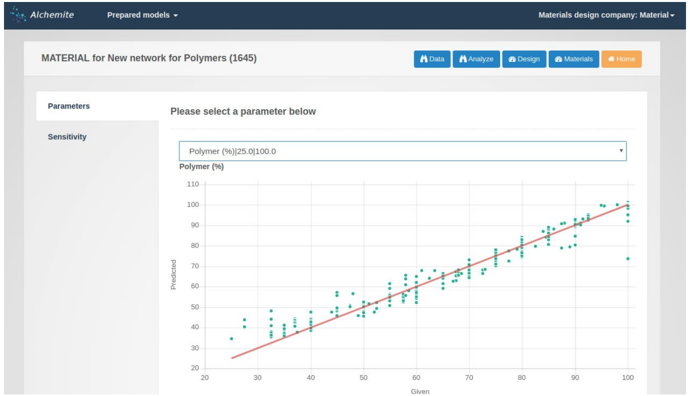
Design and interrogate new materials

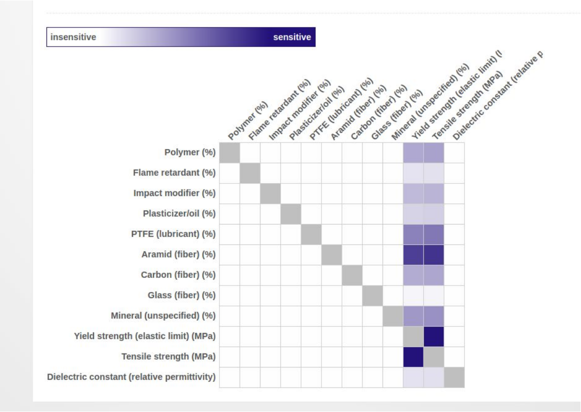




Manage and share models

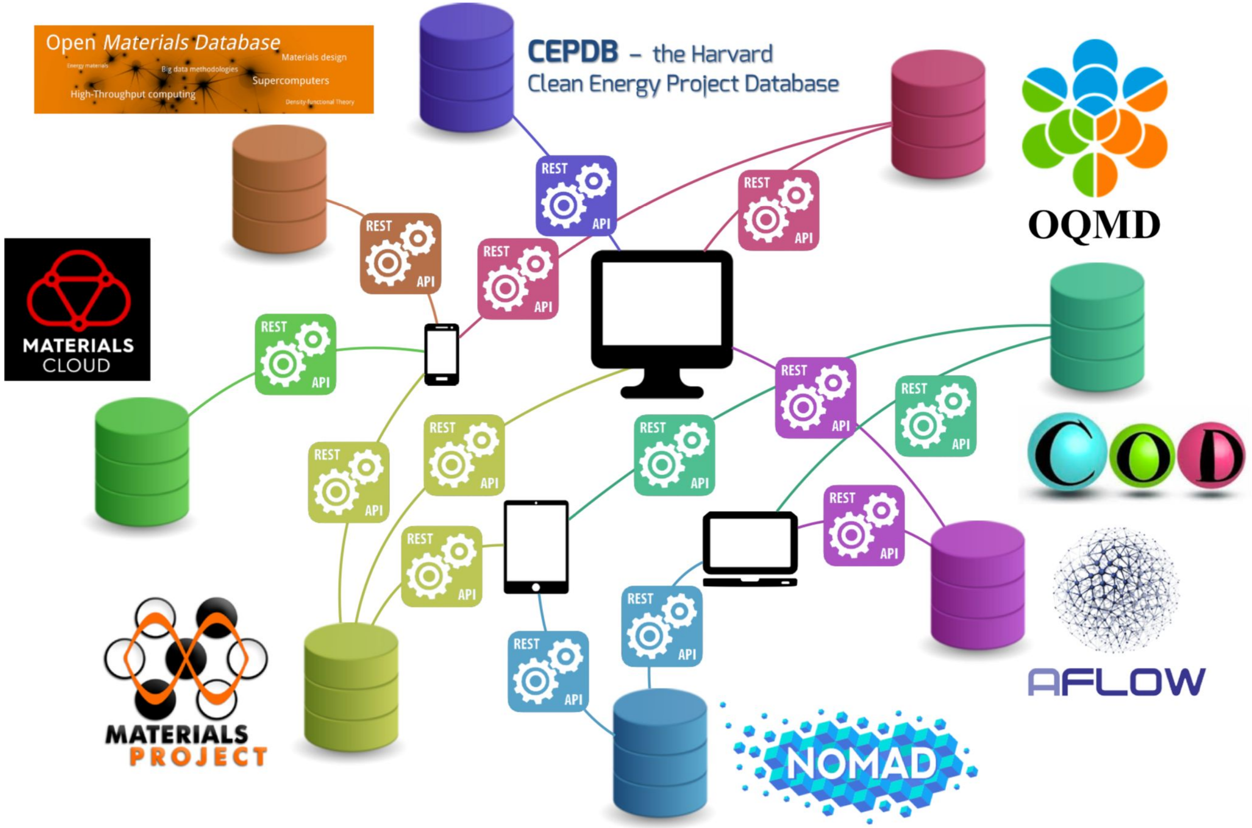




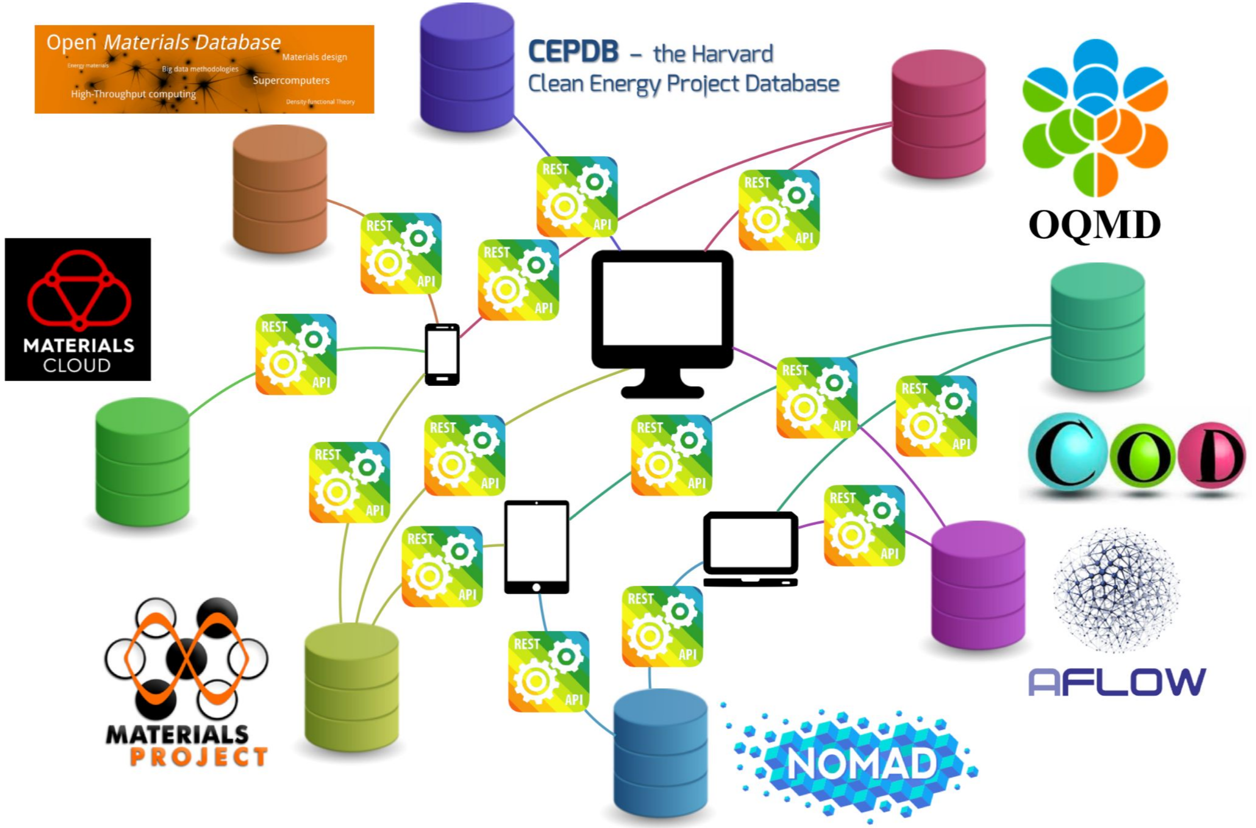


Zoo of materials databases

Labor intensive to harvest data



Universal API would ease access



OPTiMaDe

Open Databases Integration for Materials Design

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

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