UNIVERSITY OF CAMBRIDGE

Machine learning: *a priori* or *a posteriori*?

Gareth Conduit

Machine learning algorithm to

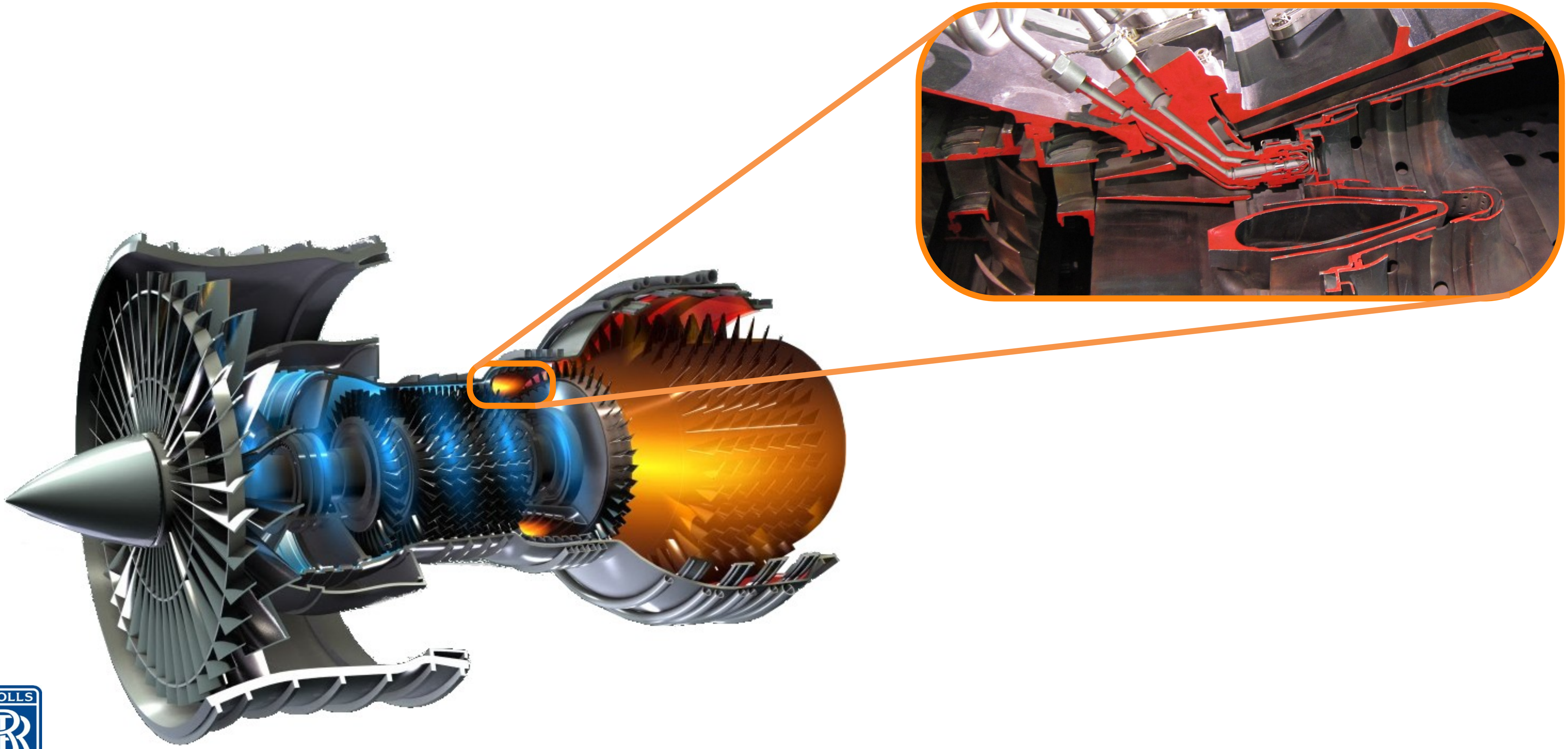
Merge *a priori* computer simulations and physical laws with *a posteriori* experimental data

Exploit *a priori* property-property correlations

Train from sparse datasets

Reduce costly experiments to accelerate discovery

Combustor in a jet engine

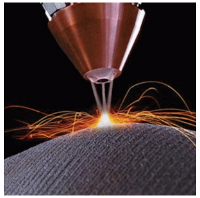


A posteriori black box machine learning for materials design

Composition

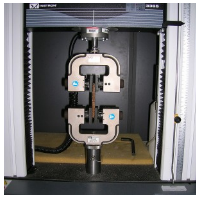
Properties

Defects

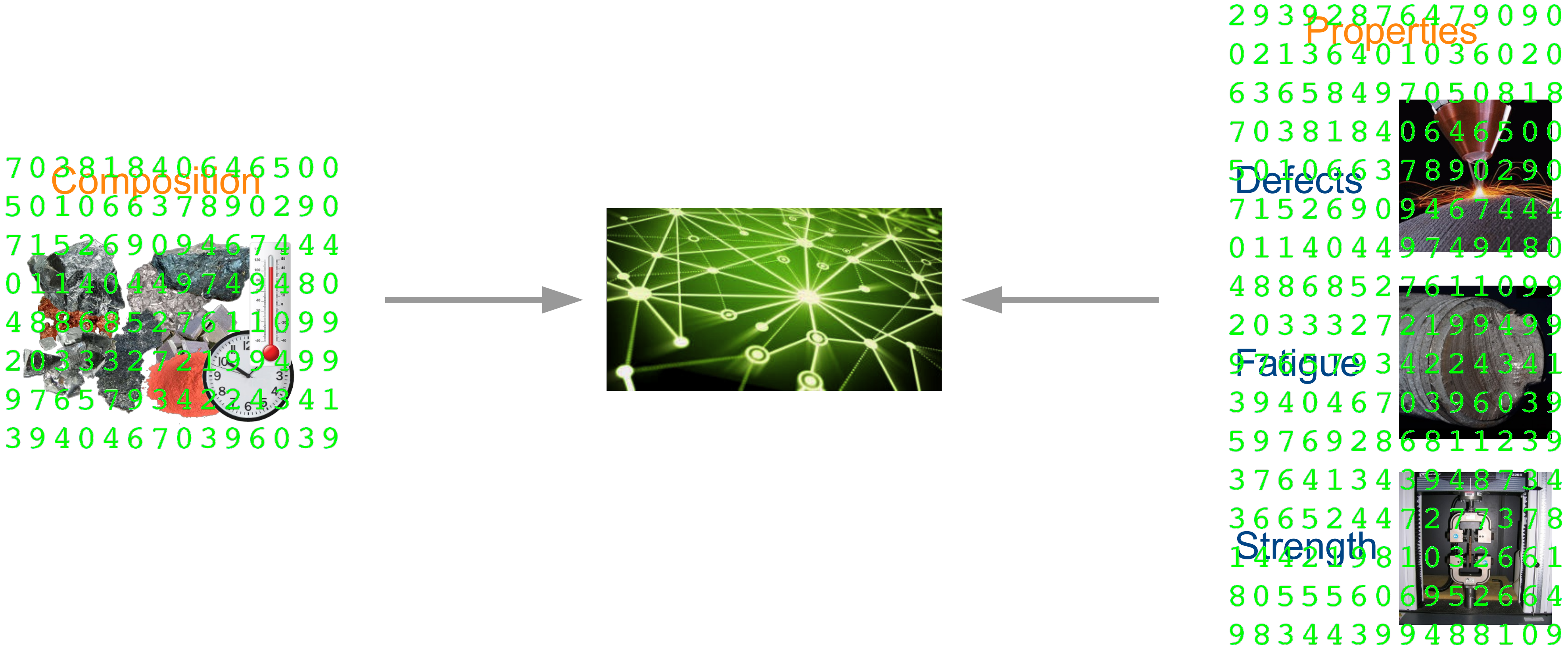


Fatigue

Strength



Train the *a posteriori* machine learning

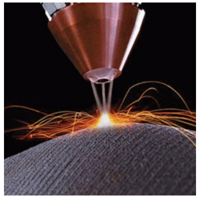


A posteriori machine learning predicts material properties

Composition

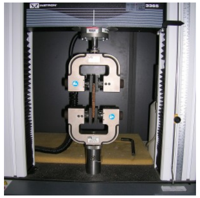
Properties

Defects



Fatigue

Strength



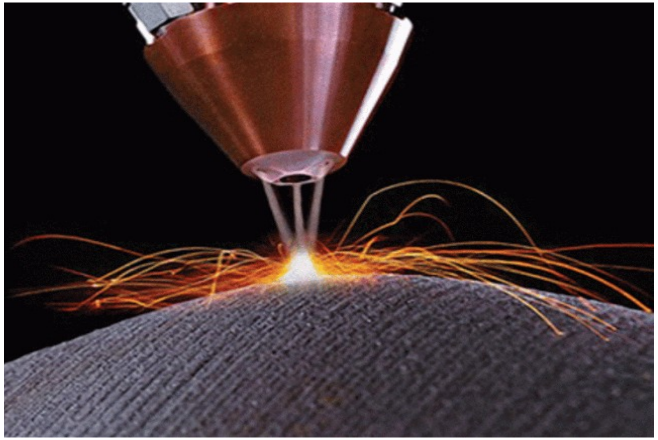
Data available to model defect density

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

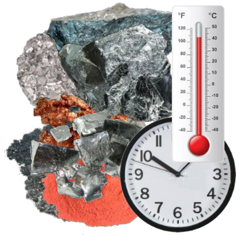
Ability for printing and welding are strongly correlated



Laser

Electricity

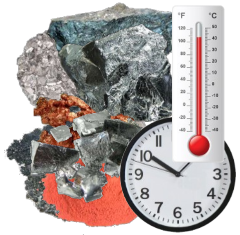
First predict weldability



1000 entries

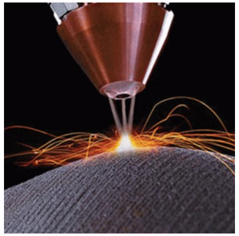
Use 1000 weldability entries to understand complex composition → weldability model

Use *a posteriori* weldability to *a priori* predict defects formed



1000 entries

10 entries



Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation

Use *a priori* CALPHAD to *a priori* predict strength

Use 100,000 CALPHAD results to model complex composition → phase behavior

500 strength entries capture the phase behavior → strength relationship

Two interpolations aid the composition → strength extrapolation

Target properties

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

Cr 19%

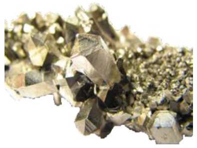
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



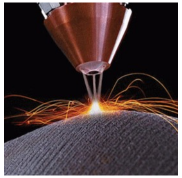
Al 2.9%

C 0.04%

B 0.01%

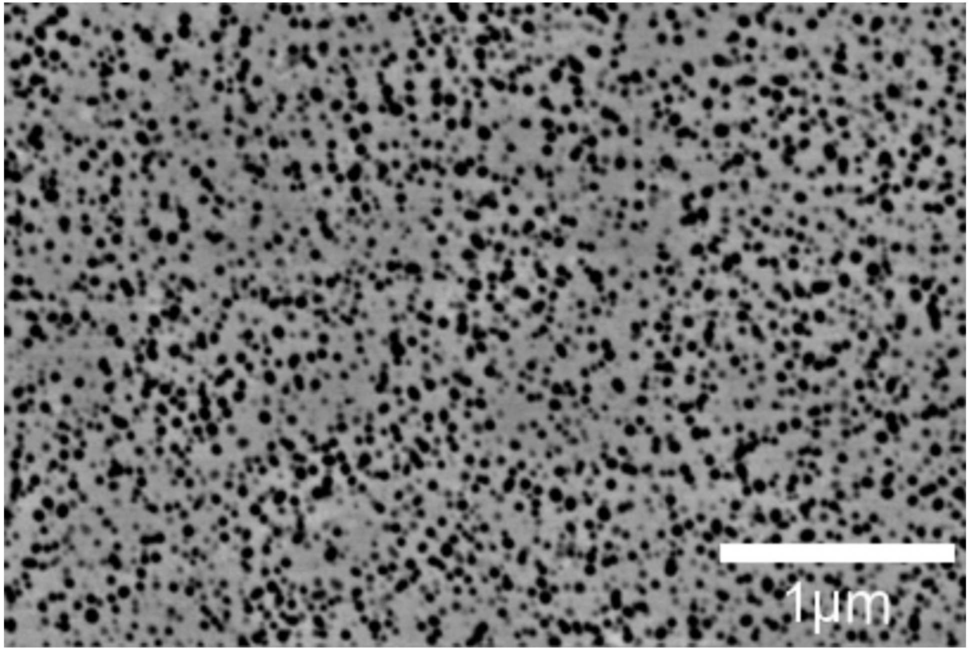
Ni

Expose 0.8

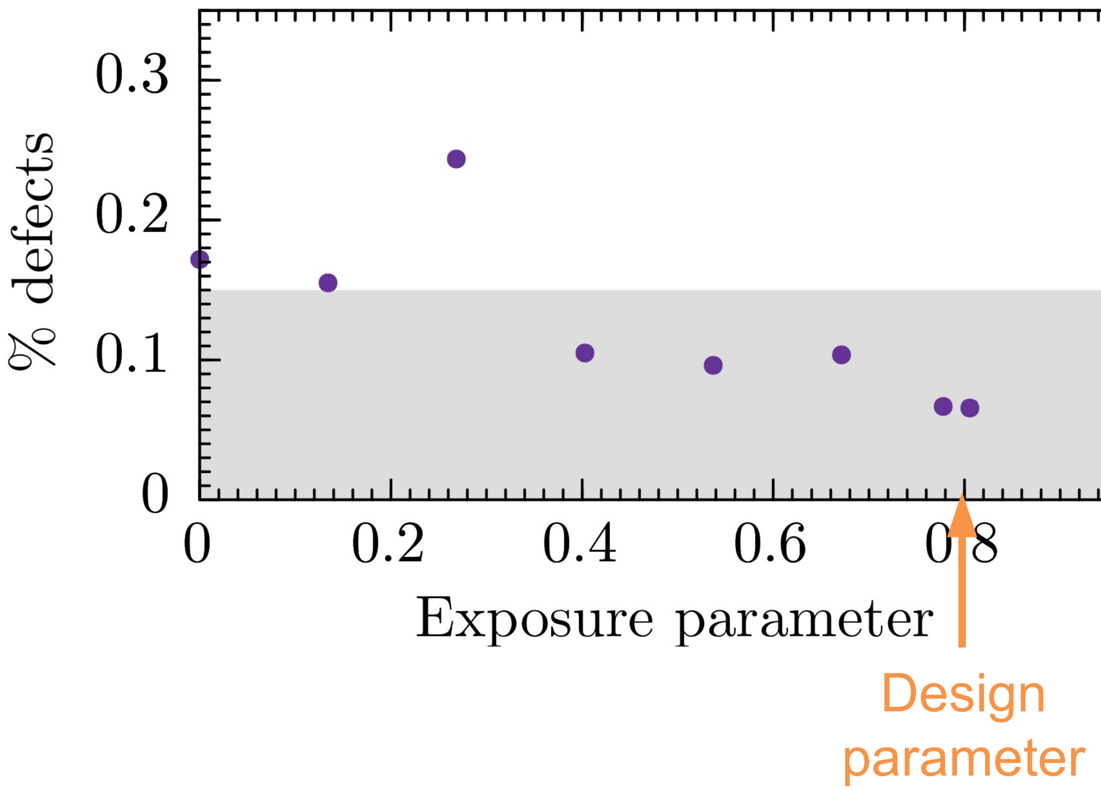


T_{HT} 1300ºC

Microstructure

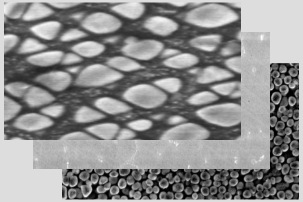


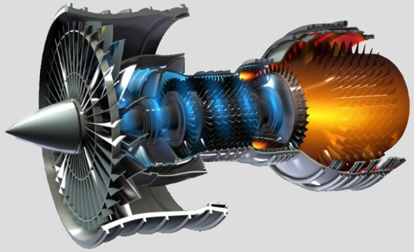
Testing the defect density



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

DOMINO

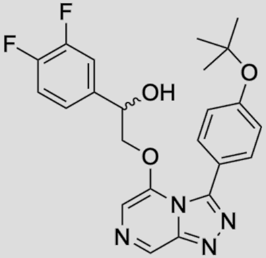




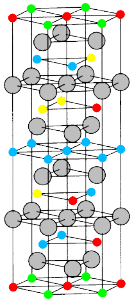
ROLLS ROYCE

BOEING

Agency for Science, Technology and Research
SINGAPORE



e-therapeutics
optibrium
Genentech
A Member of the Roche Group
University of Dundee
OSM
Constellation PHARMACEUTICALS
zoetis
Celgene
MILLENNIUM PHARMACEUTICALS, INC
Janssen
Takeda
SANOFI
AstraZeneca



SAMSUNG

Commercialization

intellegens

Alchemite Analytics™ platform for materials and chemicals with Intellegens released in September 2020

optibrium

Machine learning tool embedded into Cerella™ released in October 2020

Ansys / GRANTA

Integrate machine learning into Granta MI™

Summary

Merge *a priori* computer simulations with *a posteriori* experimental data through *a priori* property-property relationships in a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Taken to market through startup Intellegens