The modern day blacksmith

Gareth Conduit
Alchemite™, a unique neural network algorithm to

Train from **sparse** datasets

**Merge** simulations, physical laws, and experimental data

**Reduce** the need for expensive experimental development

**Accelerate** materials and drugs discovery

**Generic** with **proven** applications in materials discovery and drug design
Problem statement: materials for a jet engine
Combustor in a jet engine
Direct laser deposition requires new alloys
Target properties

Elemental cost < 25 $kg\(^{-1}\)
Density < 8500 kgm\(^{-3}\)
\(\gamma'\) content < 25 wt%
Oxidation resistance < 0.3 mgcm\(^{-2}\)
Processability < 0.15% defects
Phase stability > 99.0 wt%
\(\gamma'\) solvus > 1000°C
Thermal resistance > 0.04 KΩ\(^{-1}\)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
Neural networks for materials design

Composition

Properties
- Process
- Fatigue
- Welding
Neural networks for materials design

Composition

Properties
- Process
- Fatigue
- Welding
Neural networks for materials design

Laser

Electricity
Neural networks for materials design

Composition

Properties
- Process
- Fatigue
- Welding
Neural networks for materials design
Composition

- 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
- $T_{HT} 1300^\circ C$
Microstructure
Strength comes from texture like concrete
Testing the processability: horizontal printing

![Graph showing the relationship between exposure parameter and percentage defects. The y-axis represents the percentage defects ranging from 0 to 0.3, and the x-axis represents the exposure parameter ranging from 0 to 1. The graph displays several data points indicating a trend.]

Design parameter
Testing the oxidation resistance

![Graph showing mass gain over time for C263 and AlloyDLD](image-url)
Printing components for an engine
Materials designed

Nickel and molybdenum

Experiment and DFT for batteries

Steel for welding
Founding of Intellegens

Successful projects as academic, co-founded Intellegens alongside software engineer Ben Pellegrini.

InnovateUK enabled first stage of productization.

Support from angel Graham Snudden and University of Cambridge.

Offer advanced machine learning, first perform consultancy project, then move to product.
Quantitative structure-activity relationships

Molecular weight = 183 Da
Roadmap to productization

Reseller agreement with drug discovery software company **Optibrium**

Machine learning tool embedded into next generation of Optibrium software for release in **October 2020**

**InnovateUK** award enables collaboration with Medicine Discovery Catapult
Platform: unique ability to merge different experimental quantities and computer simulations into a holistic design tool

Experience: perform consultancy projects to hone approach and gain reputation: alloy for direct laser deposition and complete $10^{11}$ drug database entries

Business: development of product with Optibrium