UNIVERSITY OF CAMBRIDGE

Artificial intelligence – a tool for the modern-day blacksmith

Gareth Conduit

Model sparse datasets by exploiting property-property relationships

Merge data, computer simulations, and physical laws

Extract information from noise

Reduce costly experiments to accelerate discovery

Commercialized as Alchemite™ by Intellegens

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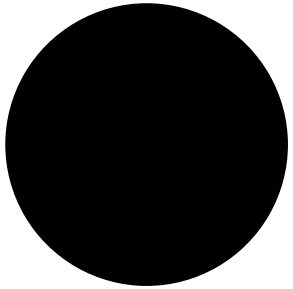
Inspired by condensed matter physics

Black box machine learning for materials design

Composition



Properties

Defects

Fatigue

Strength

Train the machine learning

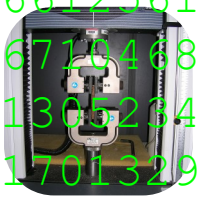
Composition

Properties

Defects

Fatigue

Strength



Machine learning predicts material properties

Composition

Properties

Defects

Fatigue

Strength

Nickel superalloys with
Rolls Royce University Technology Centre

Dr Vadegadde Duggappa

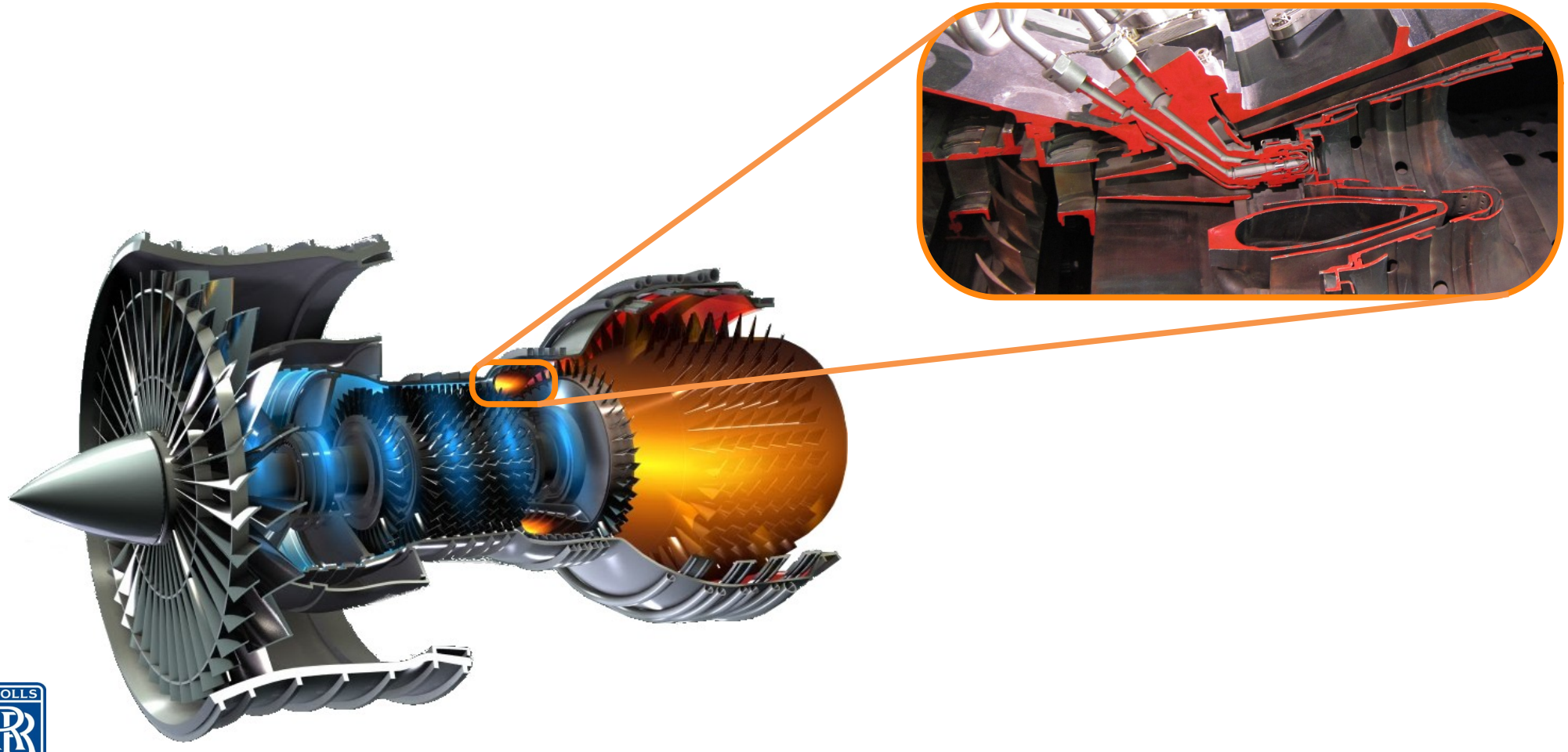
Dr Bryce Conduit

Professor Howard Stone

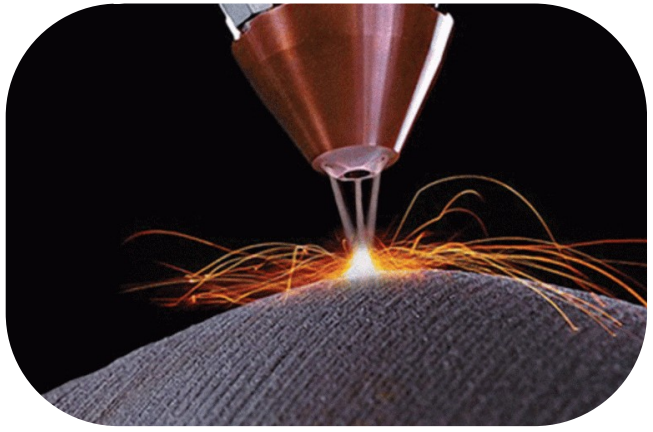
Dr Gareth Conduit

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

Combustor in a jet engine

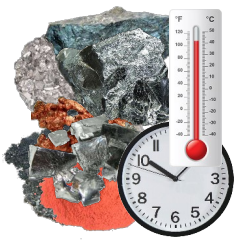


Defects form during printing



Laser

Data available to model defect density



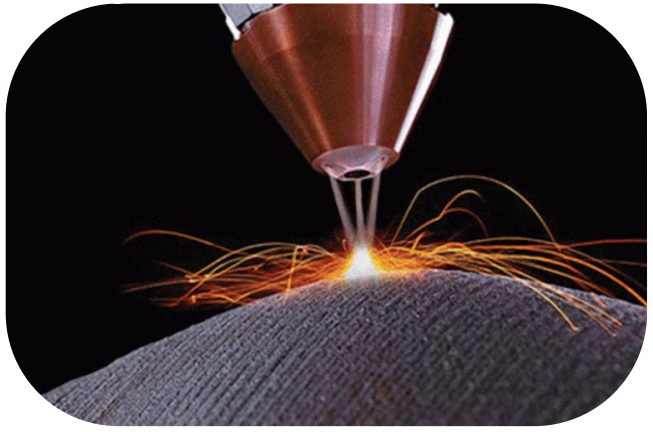
10 entries

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

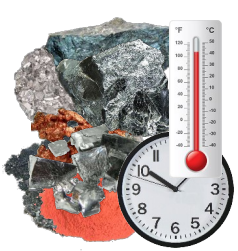
Ability for printing and welding are strongly correlated



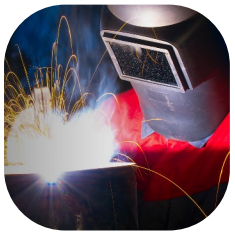
Laser

Electricity

First predict weldability

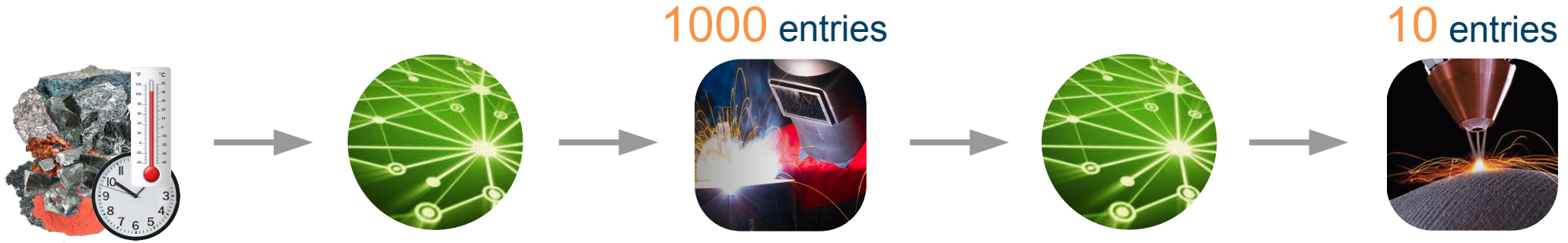


1000 entries



Use 1000 weldability entries to understand complex composition → weldability model

Use weldability to predict defects formed

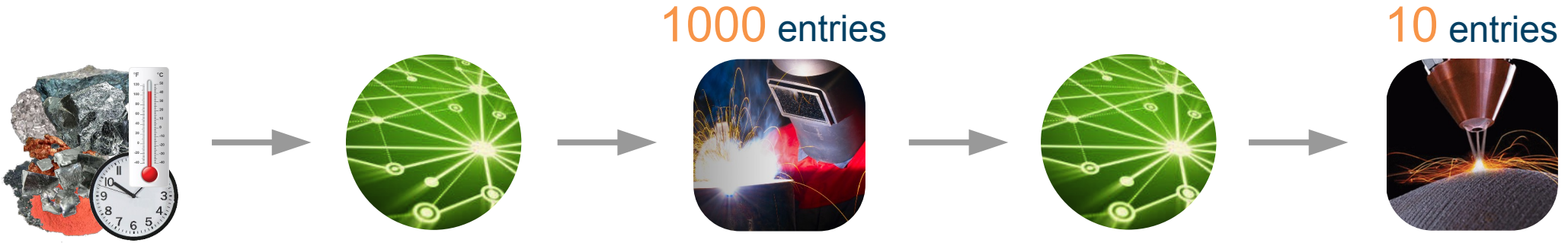


Use 1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation

Use weldability to predict defects formed



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

cf Hubbard Stratonovich transformation

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%

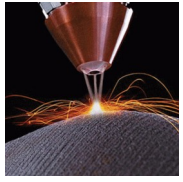
Al 2.9%

C 0.04%

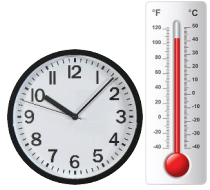
B 0.01%

Ni

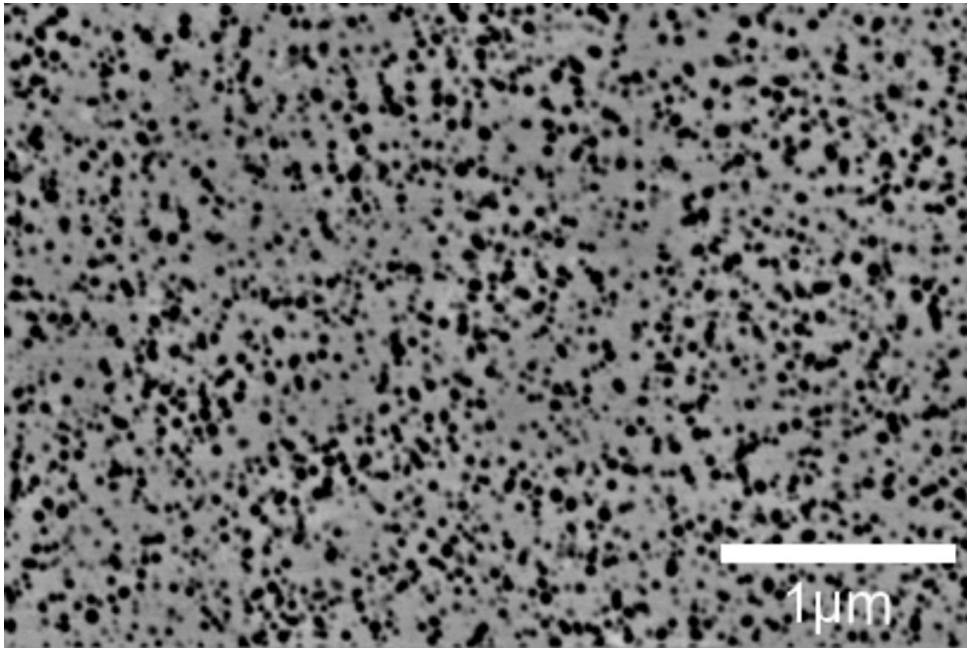
Expose 0.8



T_{HT} 1300ºC

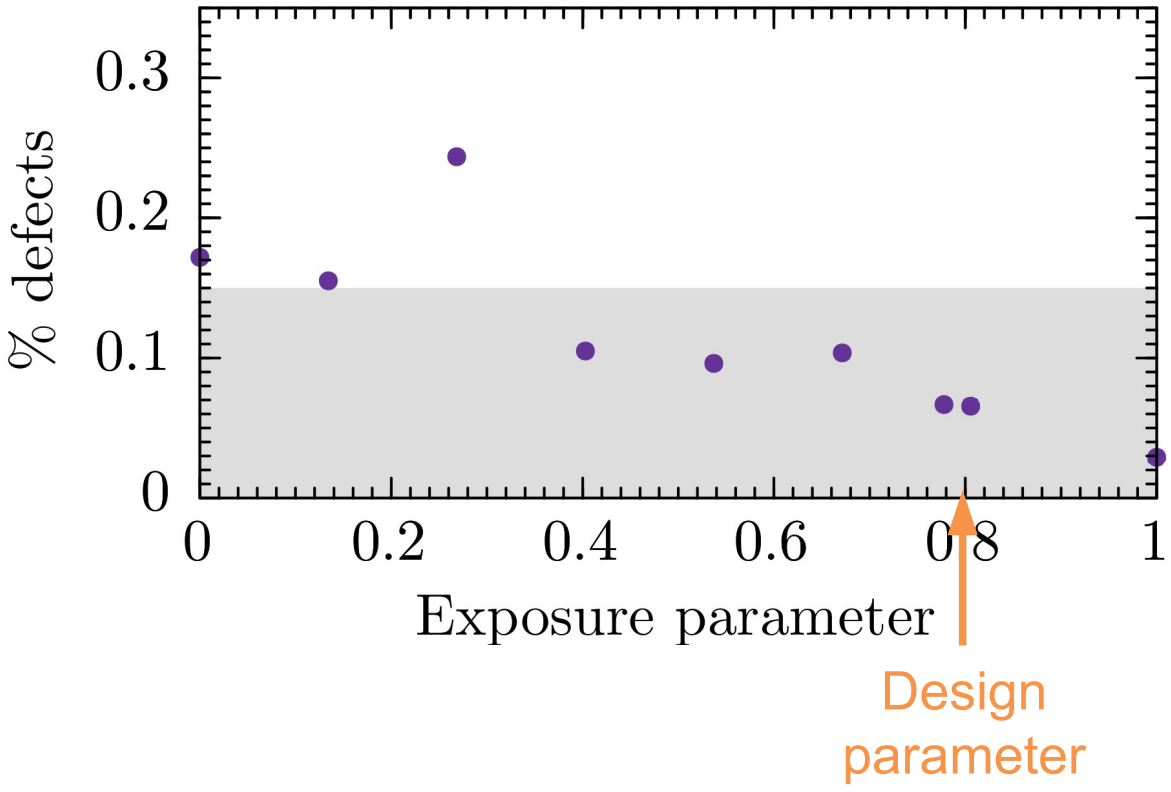


Microstructure



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

Testing the defect density



Probabilistic neural network identification of an alloy for direct laser deposition
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Development of methodology

2013

Multiple properties for Rolls Royce engines

Development of methodology

2013	2014
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP

Development of methodology

Concurrent materials design

2013	2014	2015
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship

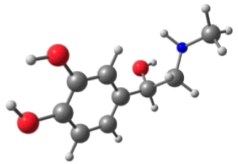
Development of methodology

Concurrent materials design

2013	2014	2015	2016
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung

Development of methodology

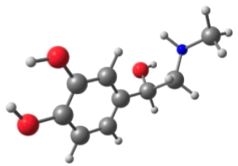
Concurrent materials design



2013	2014	2015	2016	2017
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung	Drug discovery study with etherapeutics

Development of methodology

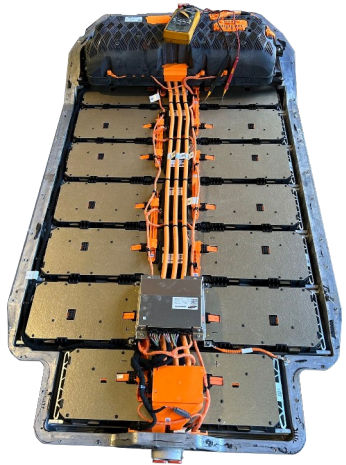
Concurrent materials design



2013	2014	2015	2016	2017	2018
Multiple properties for Rolls Royce engines	Property-property correlations with Rolls Royce and BP	Royal Society University Research Fellowship	Experiment-simulation correlations with Samsung	Drug discovery study with etherapeutics	Founding of Intellegens

Rubber renaissance

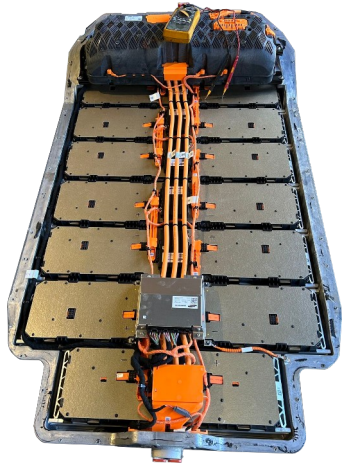
Rubber for electric vehicles



Rubber renaissance

Potential energy in elastic band

$$E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}10 \times 0.1 = 0.5\,\text{J}$$



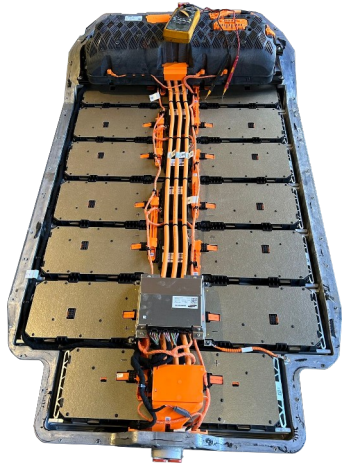
Rubber renaissance

Potential energy in elastic band

$$E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}10 \times 0.1 = 0.5\,\text{J}$$

Kinetic energy in handgun bullet

$$E = \frac{1}{2}mv^2 = \frac{1}{2}0.005 \times 300^2 = 225\,\text{J}$$



Rubber renaissance

Potential energy in elastic band

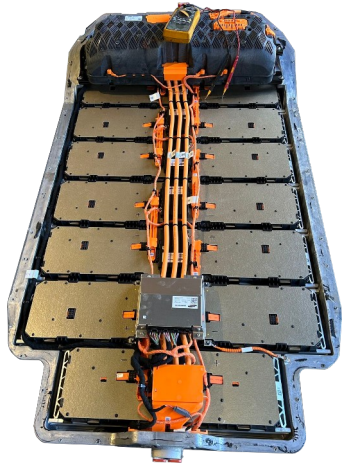
$$E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}10 \times 0.1 = 0.5\,\text{J}$$

Kinetic energy in handgun bullet

$$E = \frac{1}{2}mv^2 = \frac{1}{2}0.005 \times 300^2 = 225\,\text{J}$$

Potential energy in enormous band

$$E = \frac{1}{2}kx^2 = \frac{1}{2}Fx = \frac{1}{2}100 \times 5 = 250\,\text{J}$$



Exploit uncertainty to design concrete with

Department of Civil Engineering

Bogdan Zviazhynski

Jess Forsdyke

Professor Janet Lees

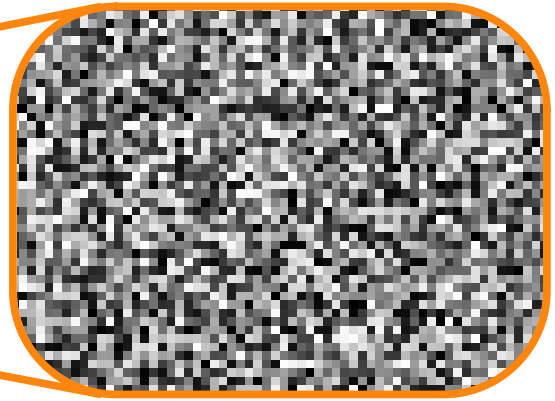
Dr Gareth Conduit

Unveil the unseen: exploit information hidden in noise
Applied Intelligence **53**, 11966 (2023)
Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

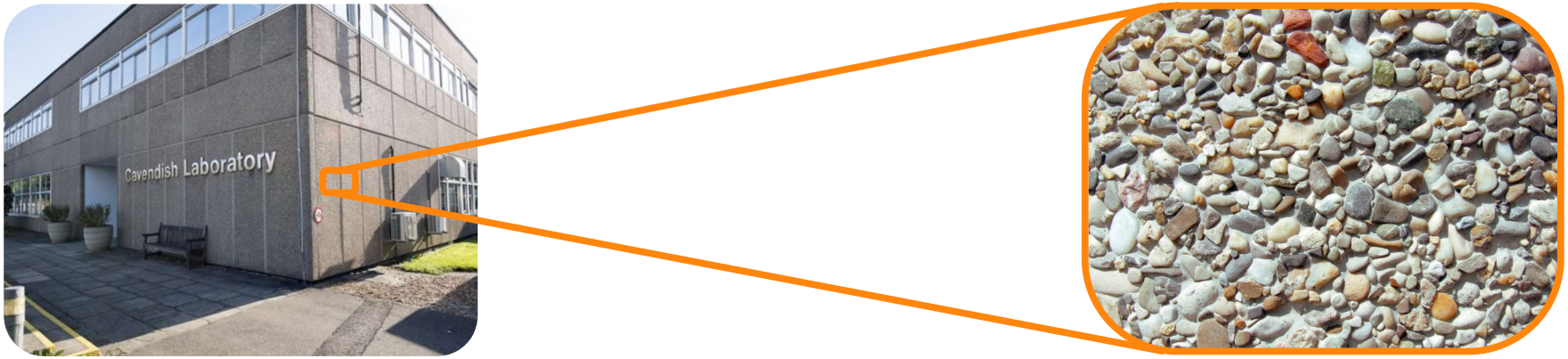
Concrete in construction

Cement & aggregate look like noise

Cement & aggregate look like noise

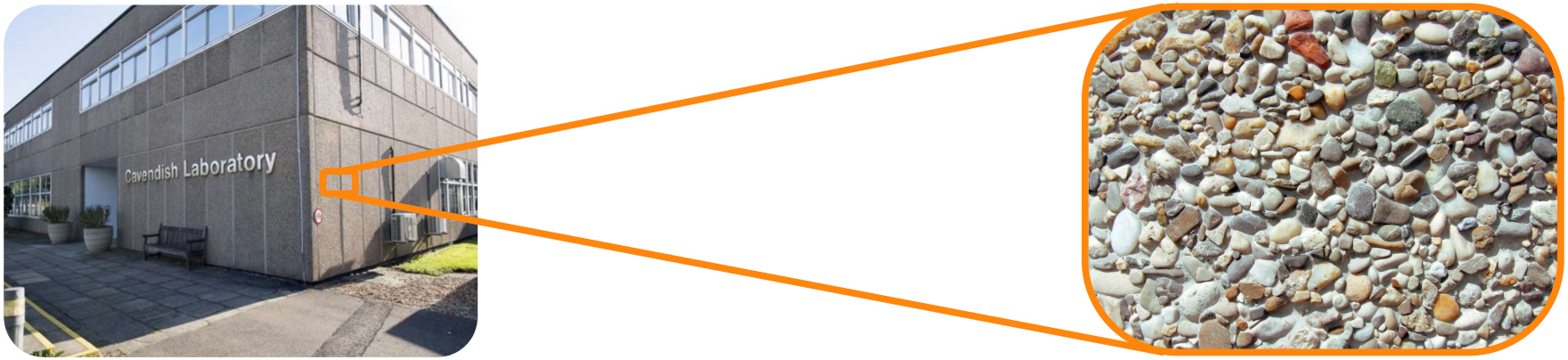


Mission



Design a concrete that is robust and environmentally friendly

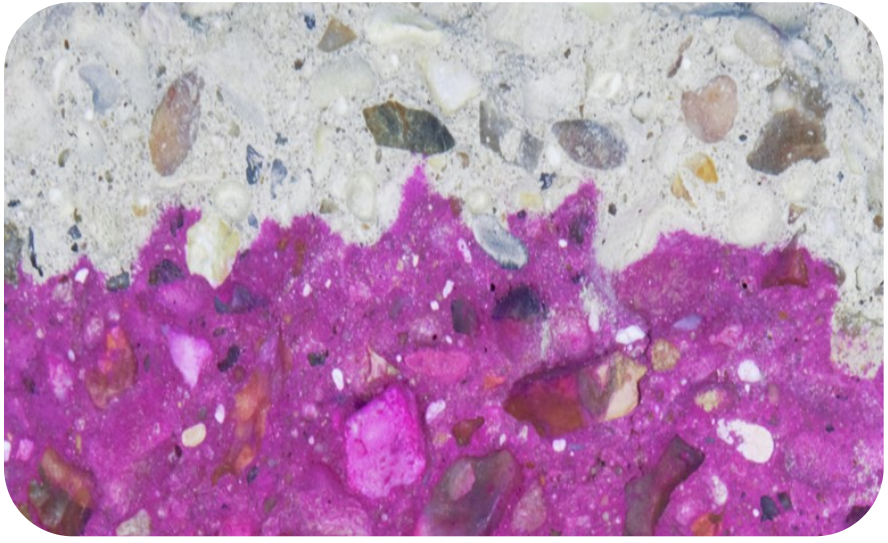
Mission



Design a concrete that is robust and environmentally friendly

Experimentally validate the concrete

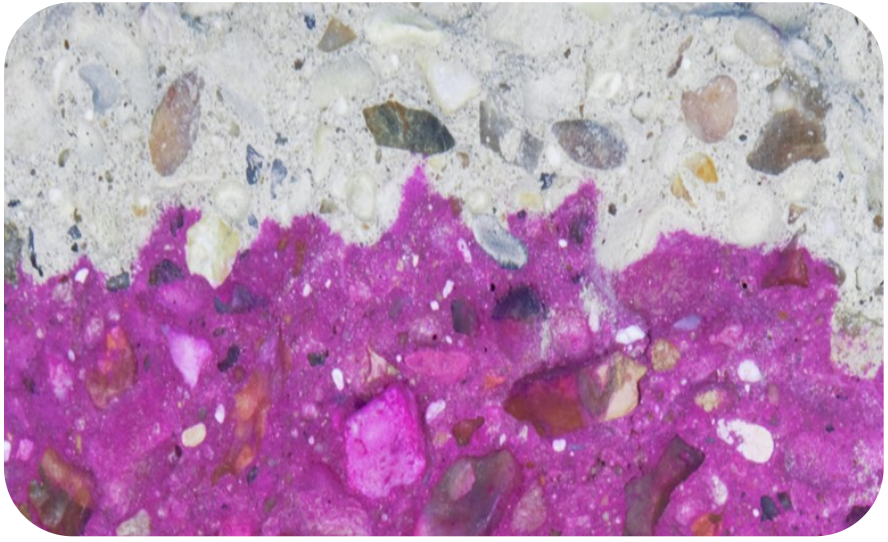
Carbonation is the probe of noise



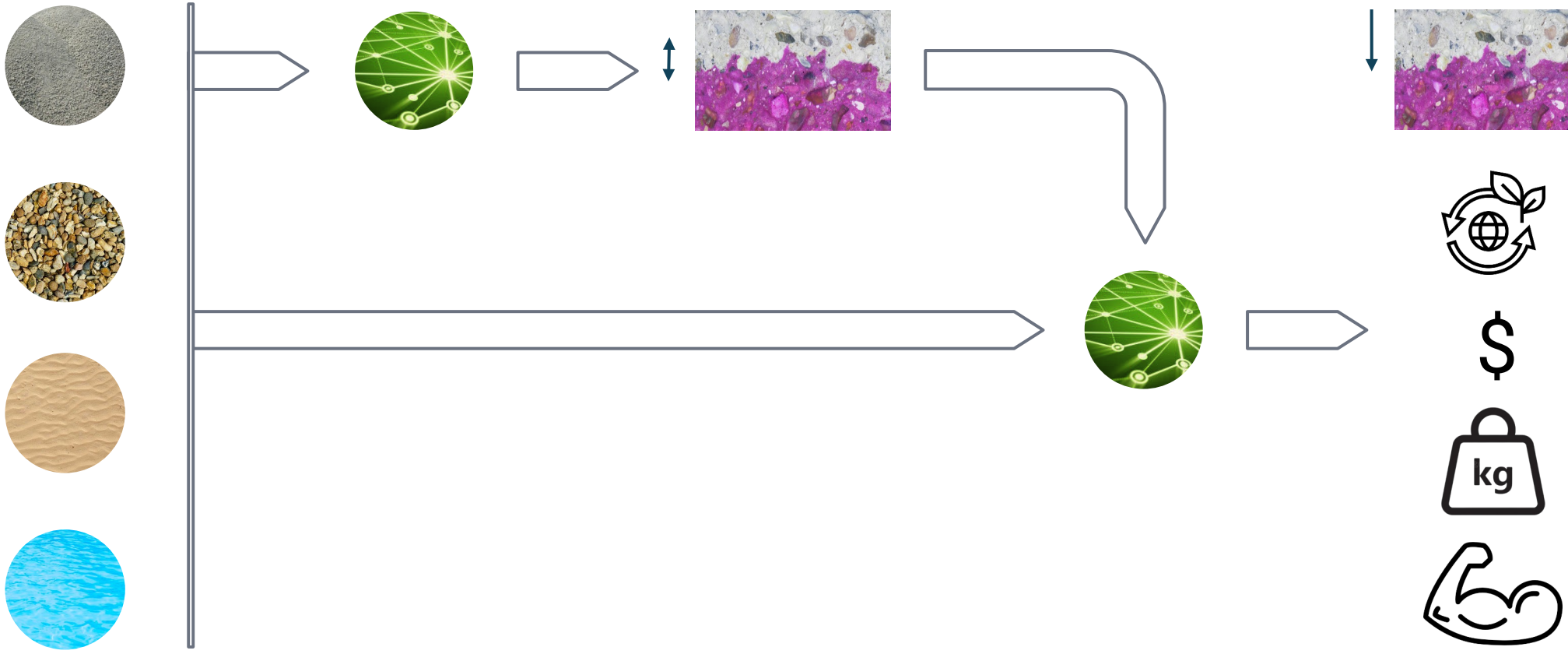
Depth and uncertainty in carbonation

Depth

Uncertainty

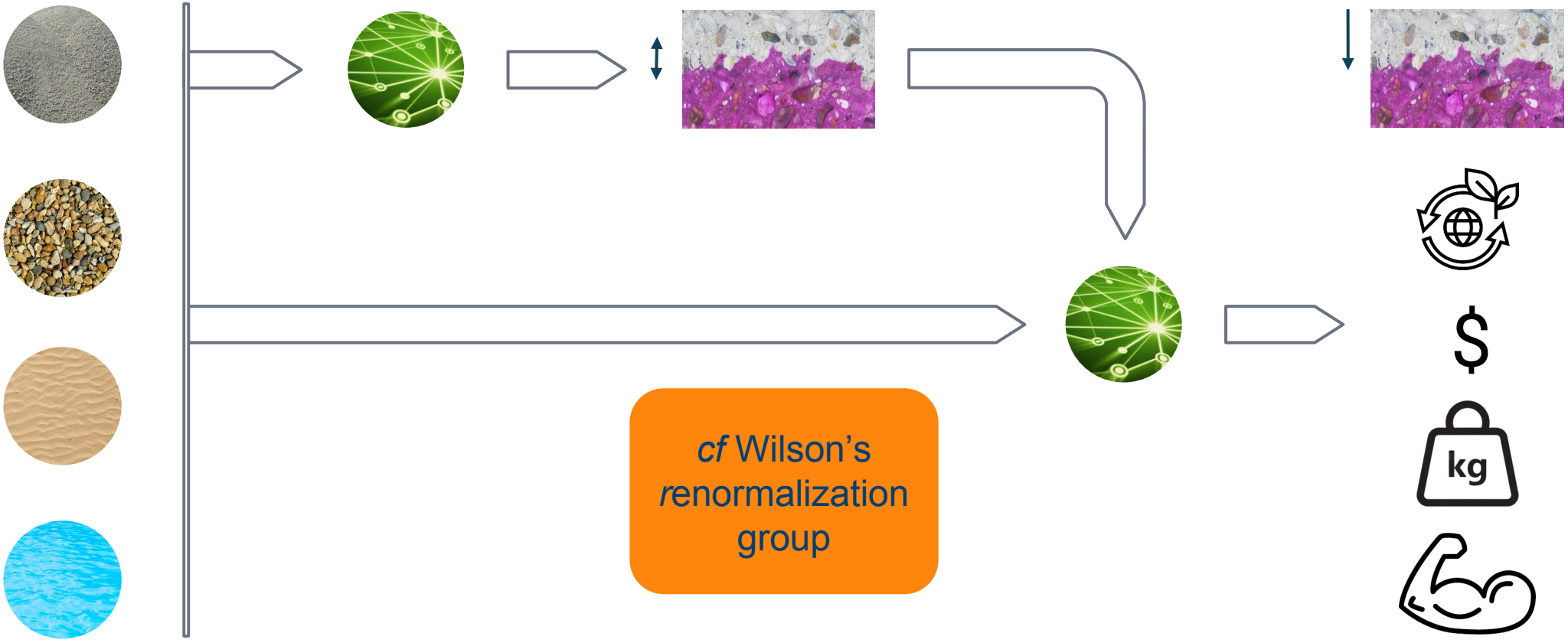


Machine learning exploits uncertainty



Unveil the unseen: exploit information hidden in noise
Applied Intelligence **53**, 11966 (2023)

Machine learning exploits uncertainty



Unveil the unseen: exploit information hidden in noise
Applied Intelligence **53**, 11966 (2023)

Concrete specification

✔ carbonation

⬇ environmental impact

✔ cost

✔ density

✔ strength

Concrete design

10.5% cement

48.4% gravel

32.6% sand

8.5% water

Concrete manufacture

Probabilistic selection and design of concrete using machine learning
Data-Centric Engineering **4**, e9 (2023)

Experimental validation of the proposed mixes

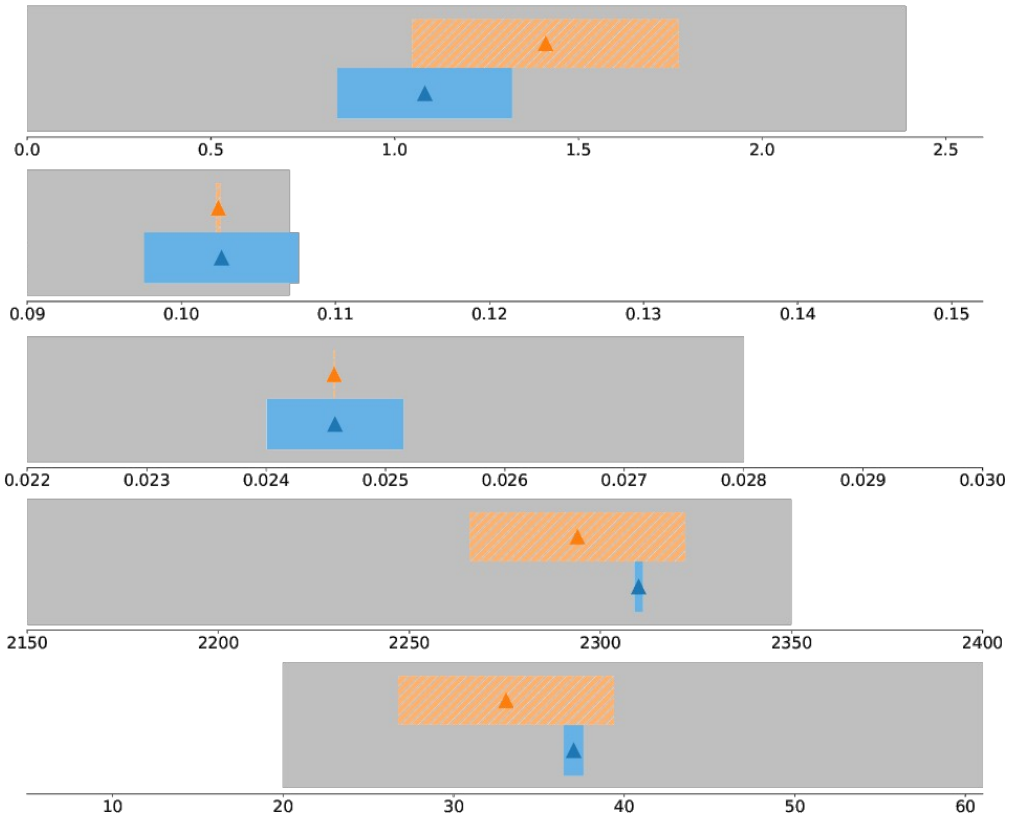
✔ carbonation

↓ environmental impact

✔ cost

✔ density

✔ strength



Experiment Model Target

Commercialization

therapeutics

bp

2018

Transfer contracts from University

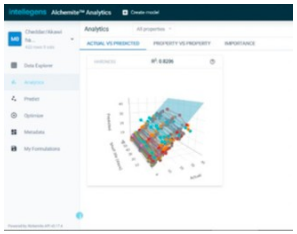
Commercialization

2018 | 2019

Transfer contracts from University

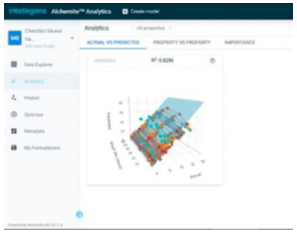
Consultancy work

Commercialization



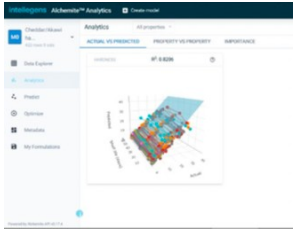
2018	2019	2020
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product

Commercialization



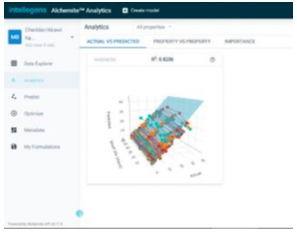
2018	2019	2020	2021
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium

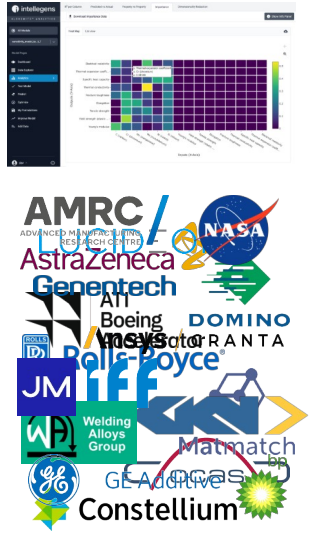
Commercialization



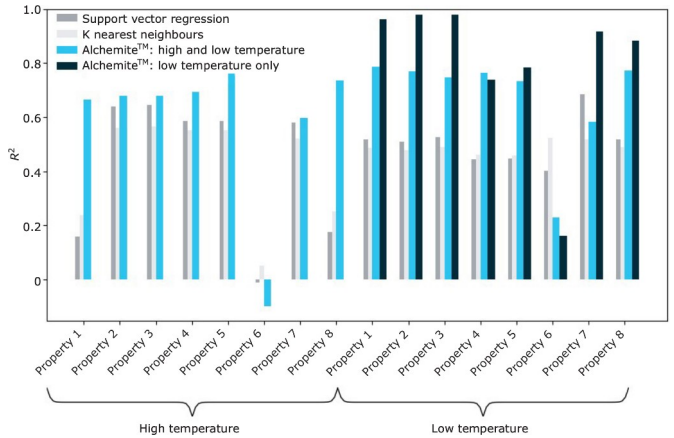
2018	2019	2020	2021	2022
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Launch product with ANSYS Granta

Commercialization

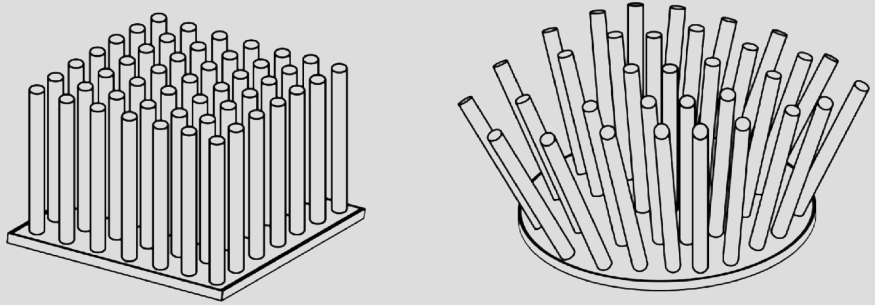




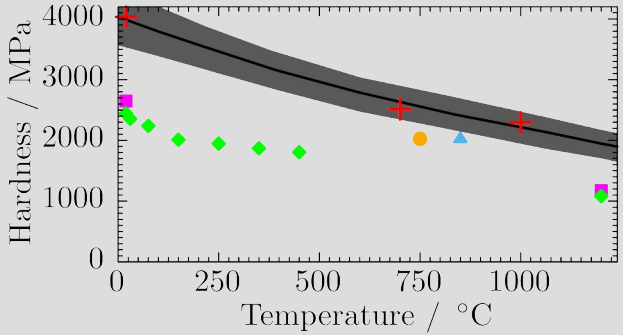
2018	2019	2020	2021	2022	2023
Transfer contracts from University	Consultancy work	Launch Alchemite Analytics™ product	Launch Cerella™ product with Optibrium	Launch product with ANSYS Granta	Enterprise licenses & healthcare market

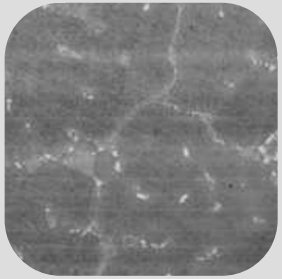


Johnson Matthey Technology Review
66, 130 (2022)



NASA Technical Memorandum
20220008637

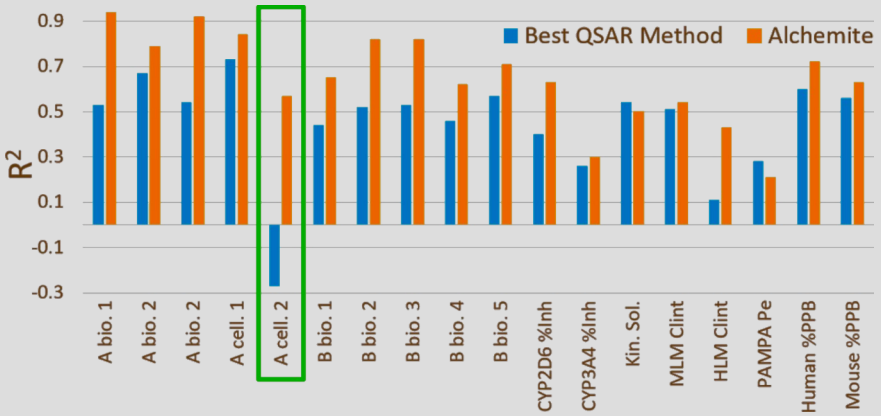




Materials & Design **131**, 358 (2017)
Scripta Materialia **146**, 82 (2018)
Data Centric Engineering **3**, e30 (2022)

Alloy	Source	ANN	Δ_σ	Actual
Steel AISI 301L	193	269	5	238[23]
Steel AISI 301	193	267	5	221[23]
Al 1080 H18	51	124	5	120[23]
Al 5083 wrought	117	191	14	300,190[4, 23]
Al 5086 wrought	110	172	11	269,131[4, 23]
Al 5454 wrought	102	149	14	124[23]
Al 5456 wrought	130	201	11	165[23]
INCONEL600	223	278	10	≥550[23]

Computational Materials
Science **147**, 176 (2018)



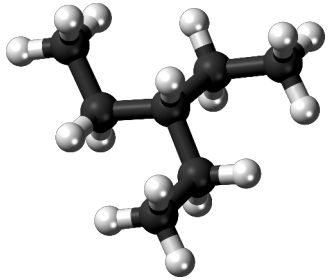
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

optibrium

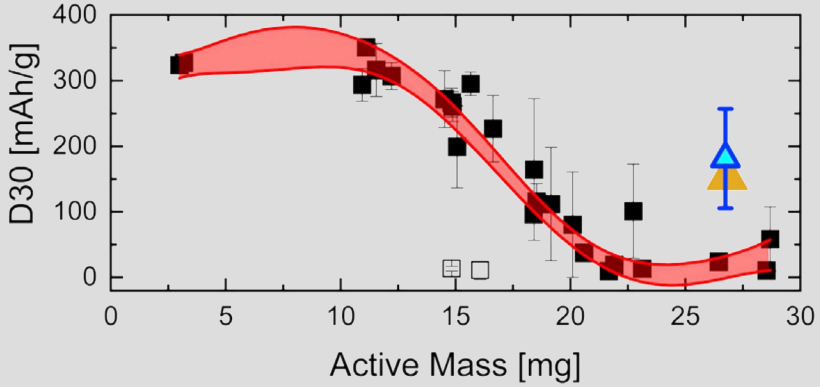
iff

Journal of Computer-Aided
Molecular Design **35**, 112501140 (2021)



Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)

bp



Nature Machine Intelligence **2**, 161 (2020)
Cell Reports Physical Science **2**, 100683 (2021)

UNIVERSITY OF BIRMINGHAM

Ansys GRANTA

Merge computer simulations with experimental data and exploit property-property relationships to circumvent missing data

Designed and experimentally verified alloy for direct laser deposition

Extract information from noise to design concrete

Generic approach applied to materials, chemicals, pharmaceuticals, and beyond

Commercialized as Alchemite™ by Intellegens