UNIVERSITY OF CAMBRIDGE

Green materials in less time: accelerate discovery with machine learning

Gareth Conduit

Model sparse datasets

Exploit property-property relationships

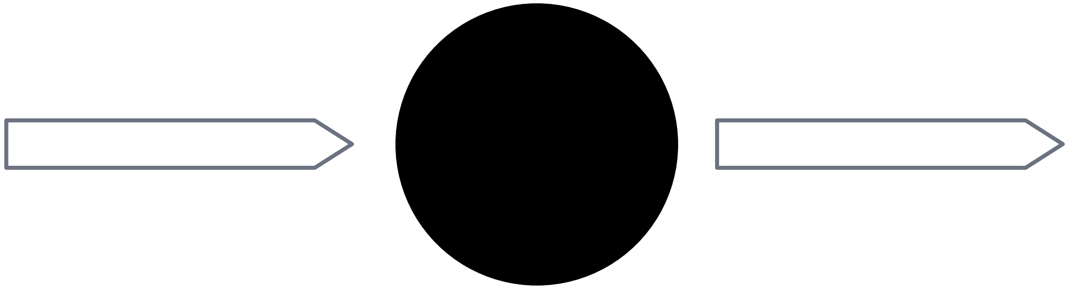
Merge data, computer simulations, and physical laws

Exploit uncertainties to deliver most robust predictions

Extract information from noise itself

Black box machine learning for materials design

Composition



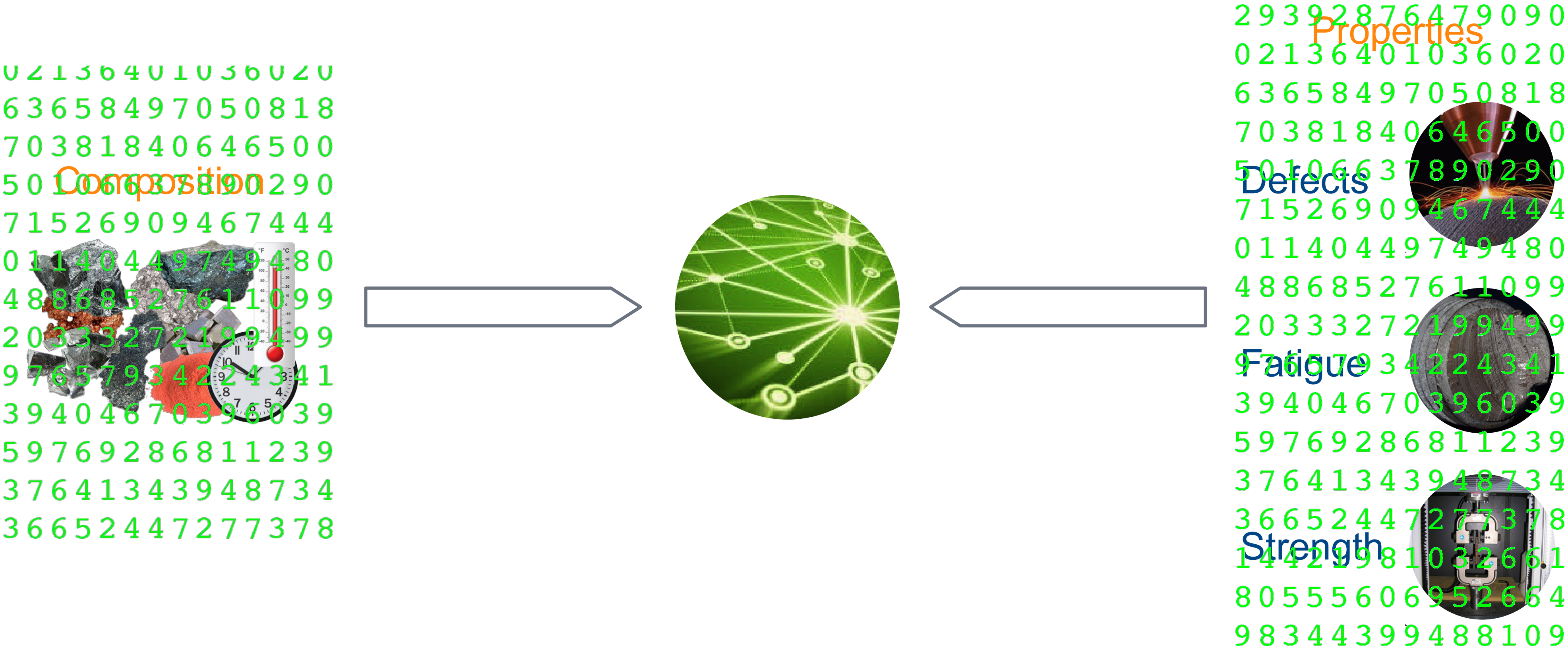
Properties

Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

Composition

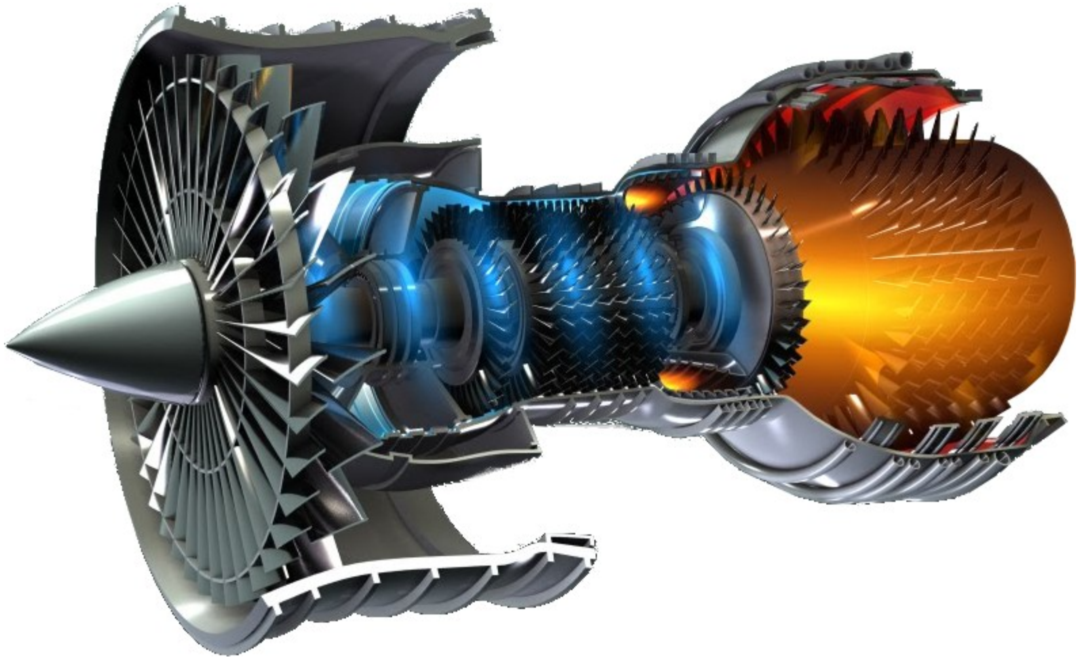
Properties

Defects

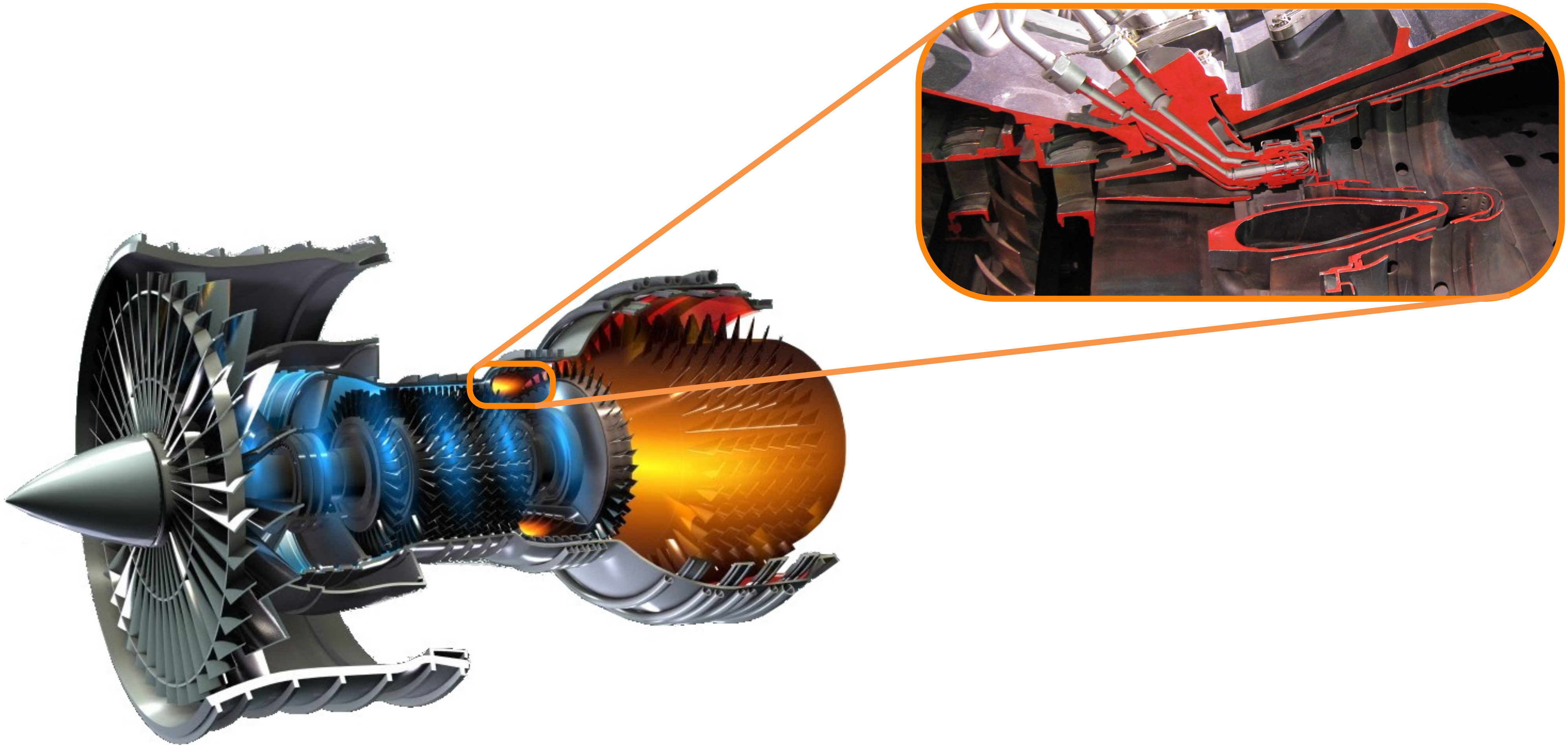
Fatigue

Strength

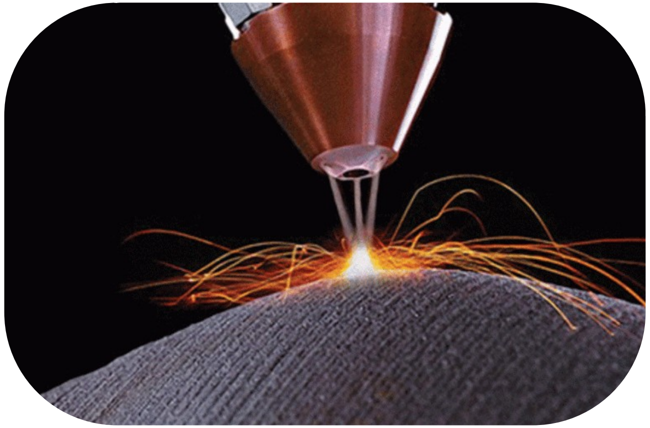
Jet engine schematic



Combustor in a jet engine



Direct laser deposition



Data available to model defect density

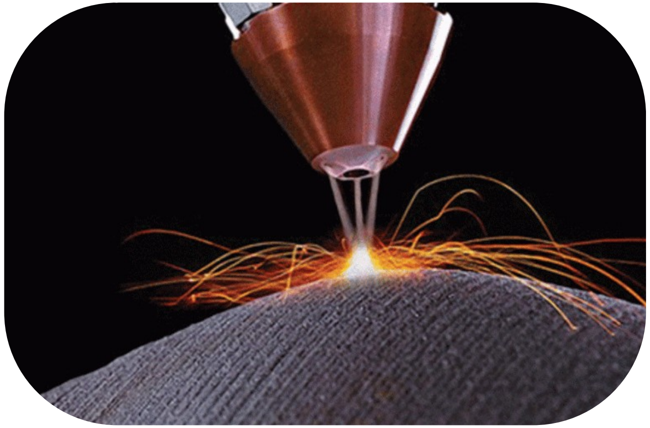
10 entries

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

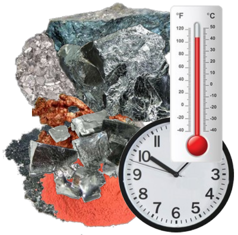
Ability for printing and welding are strongly correlated



Laser

Electricity

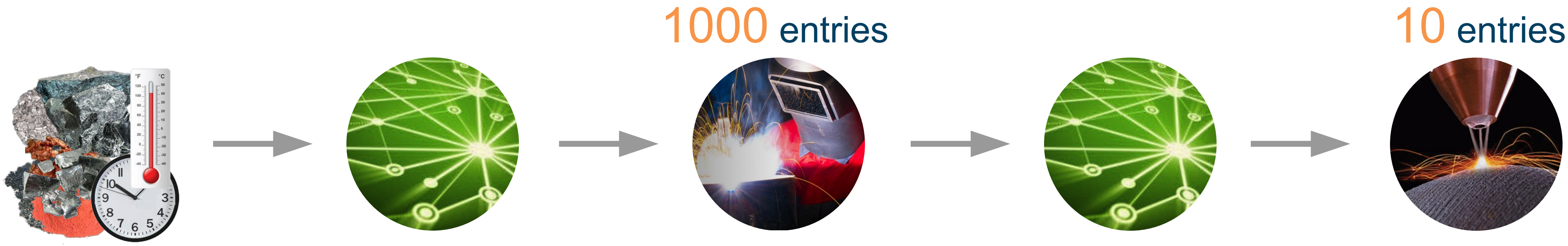
First predict weldability



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 aid composition → defects extrapolation

Use CALPHAD to predict strength

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

SCM
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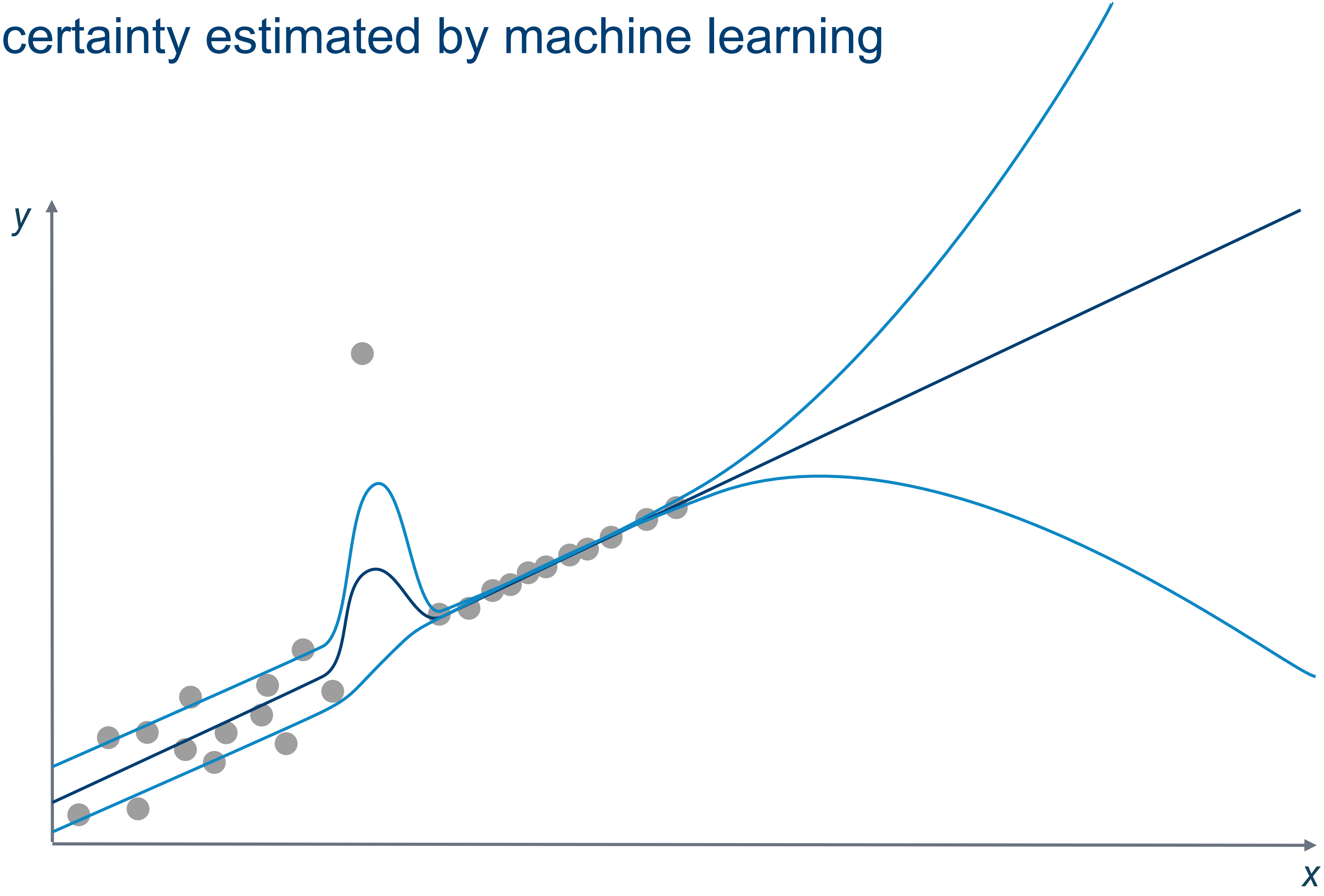
Uncertainty estimated by machine learning



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%

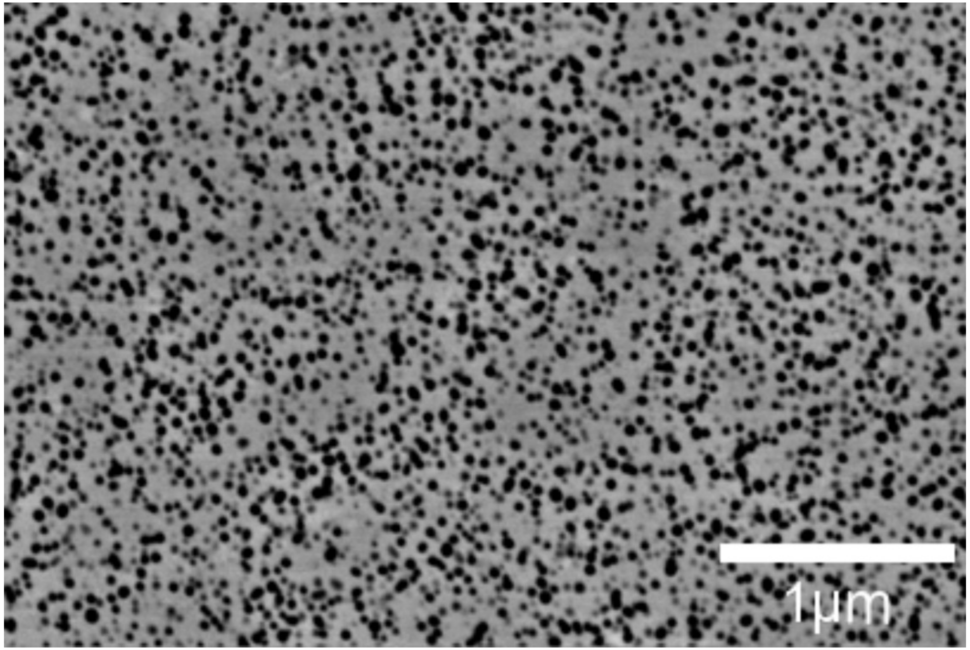
B 0.01%

Ni

Expose 0.8

T_{HT} 1300ºC

Microstructure



Probabilistic neural network identification of an alloy for direct laser deposition

B. Conduit, T. Illston, S. Baker, D. Vadegadde Duggappa, S. Harding, H. Stone & GJC

Materials & Design **168**, 107644 (2019)

Defects target

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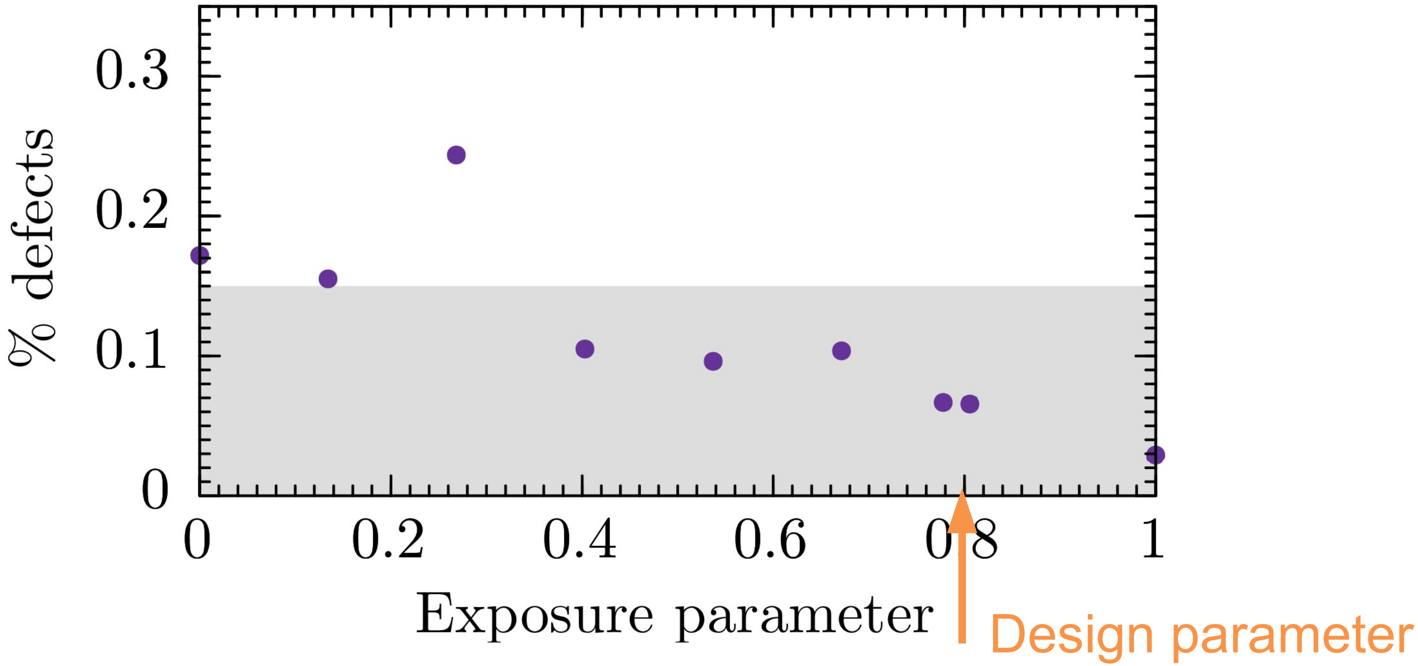
Testing the defect density



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Materials & Design **168**, 107644 (2019)

Extract and exploit uncertainty to design concrete

Bogdan Zviazhynski

Jess Forsdyke

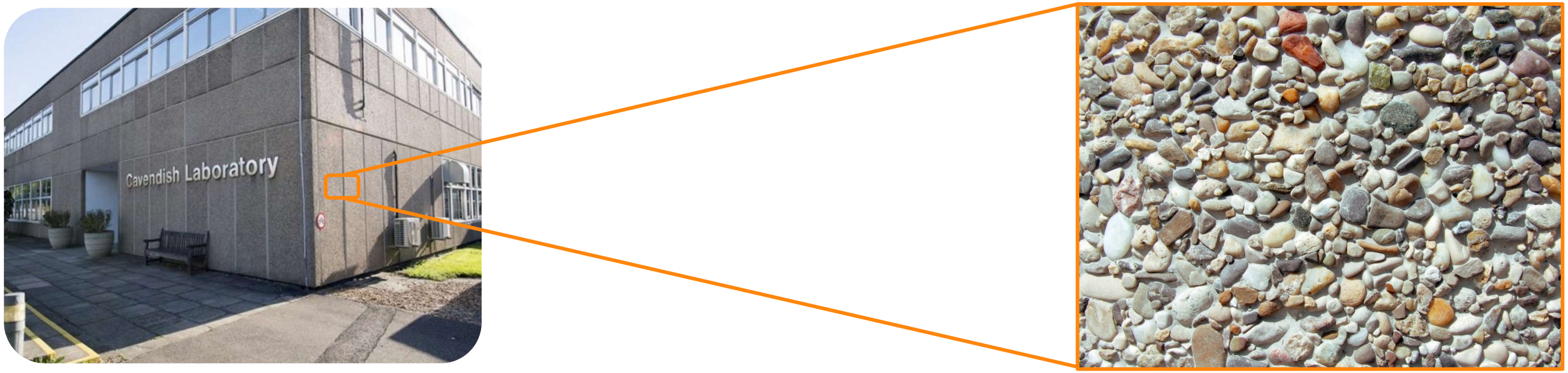
Professor Janet Lees

Unveil the unseen: exploit information hidden in noise, BZ & GJC, Applied Intelligence (2022)

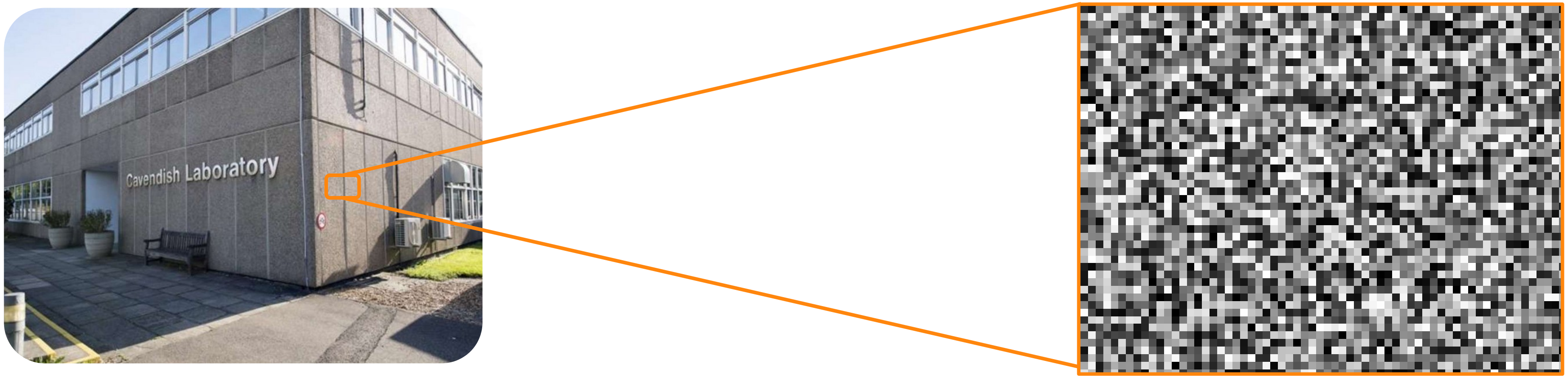
Probabilistic selection and design of concrete using machine learning
JCF, BZ, JML & GJC, Data-Centric Engineering **4**, e9 (2023)

Concrete in construction

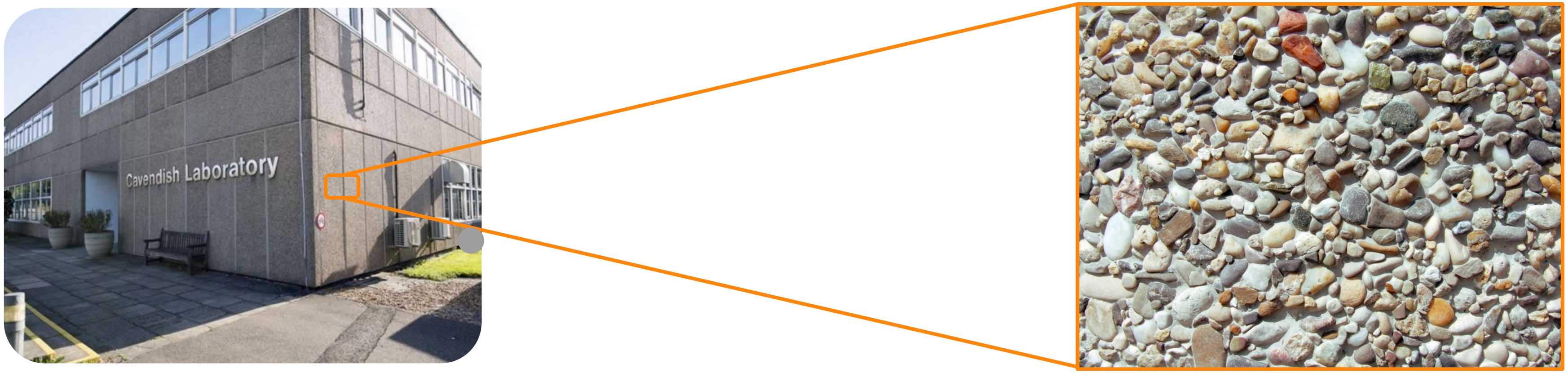
Cement & aggregate look like noise

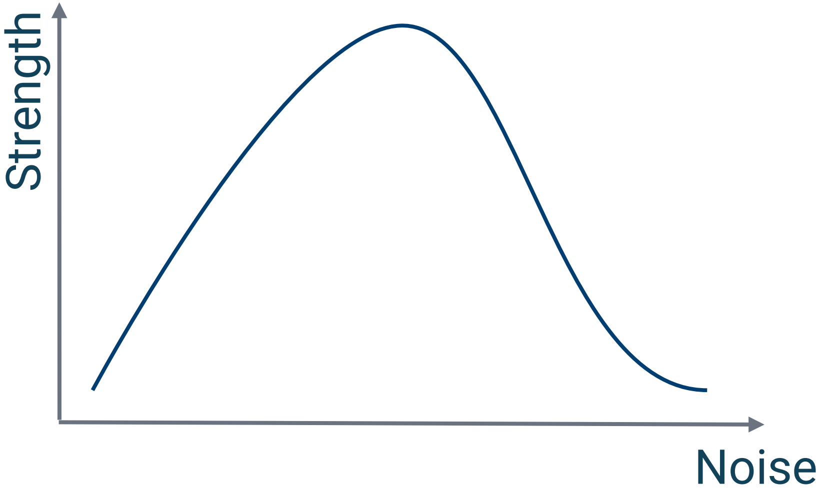


Cement & aggregate look like noise

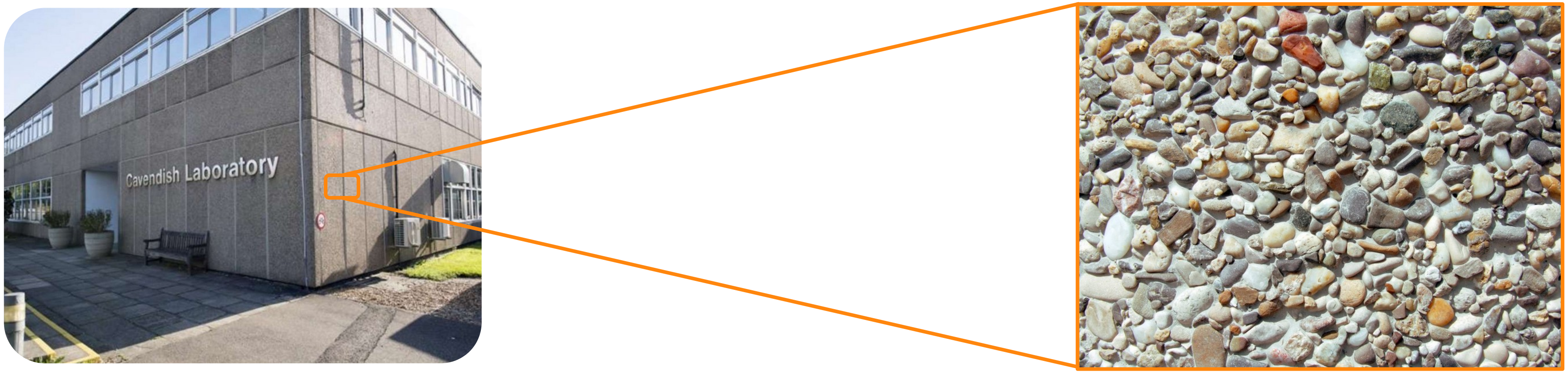


Strength is related to noise



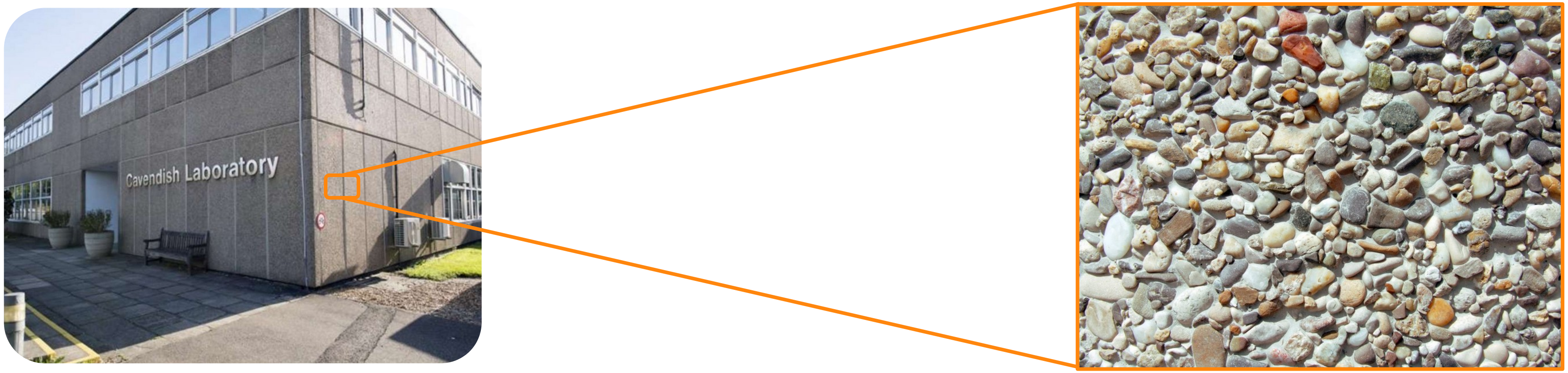


Mission



Design environmentally friendly concrete

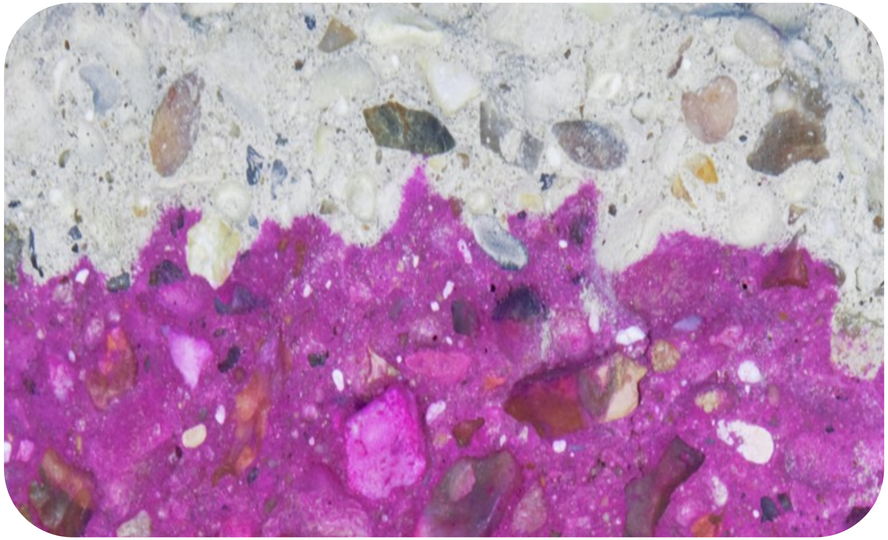
Mission



Design environmentally friendly concrete

Experimentally validate the concrete

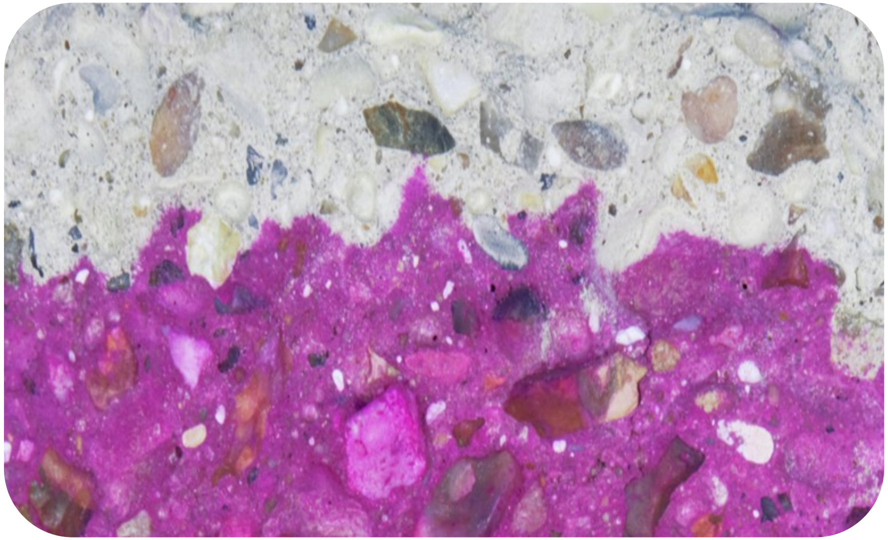
Carbonation is the probe of noise



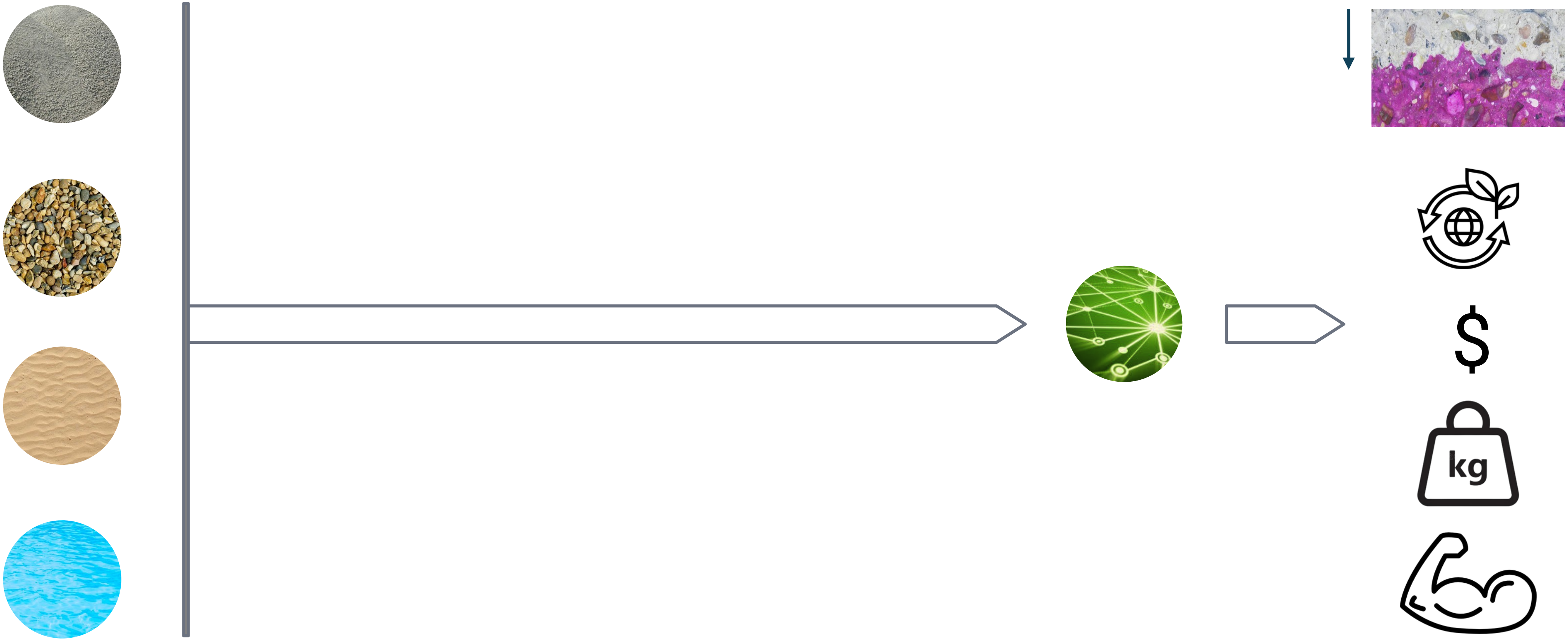
Depth and uncertainty in carbonation

Depth

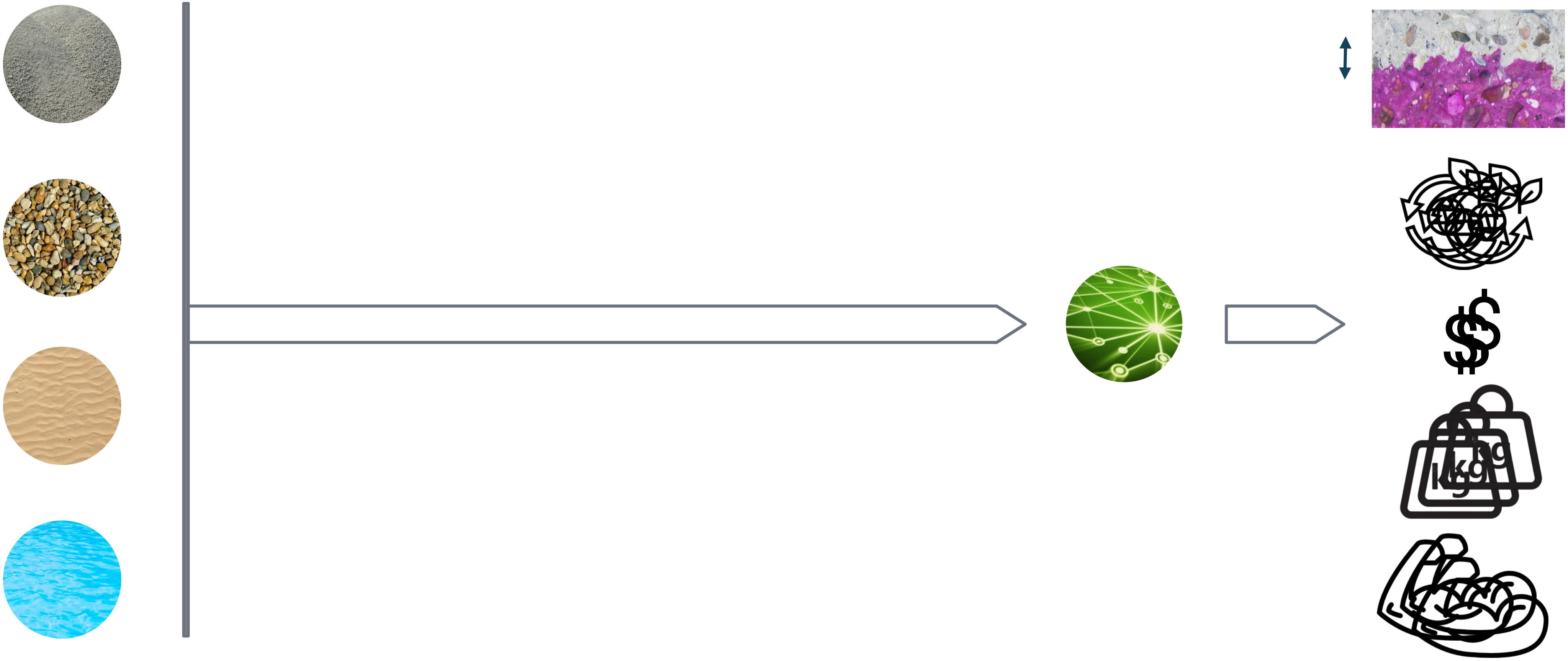
Uncertainty



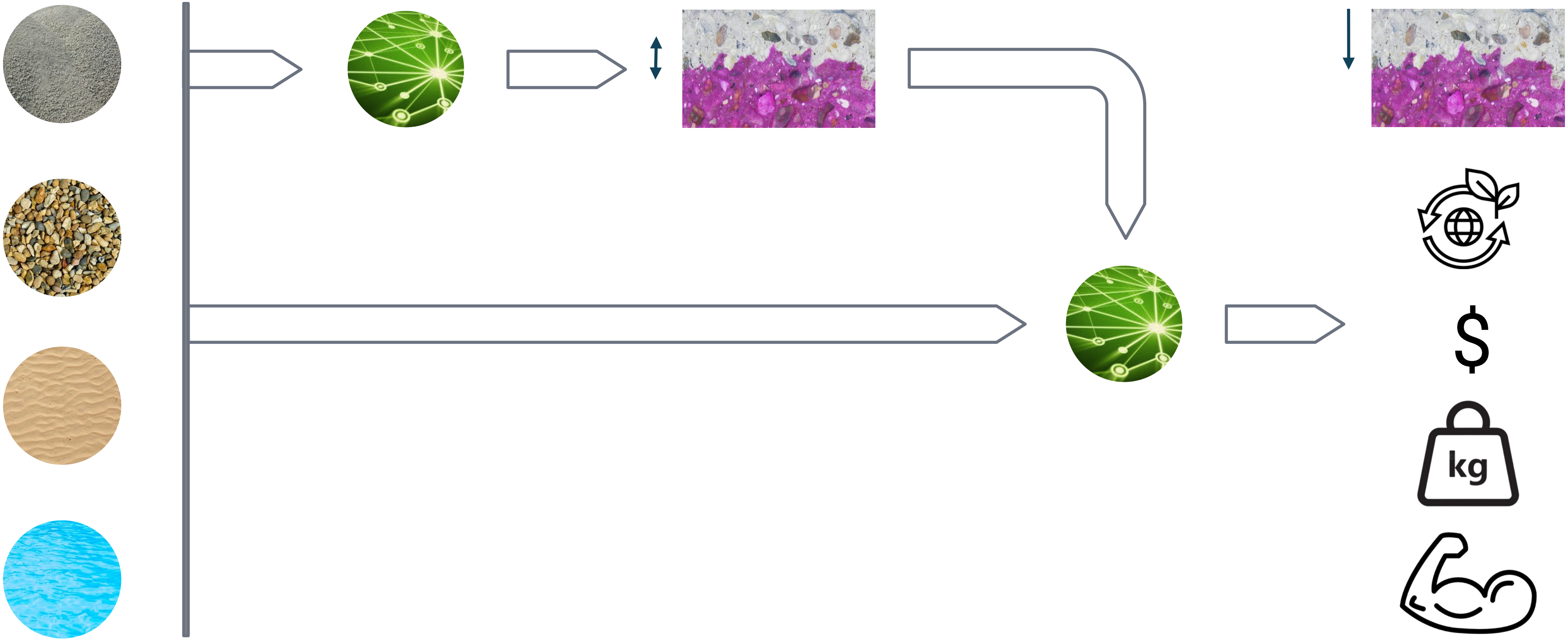
Standard machine learning predicts expectation values



Exploit machine learning uncertainty estimates for robust designs



Machine learning exploits uncertainty



Unveil the unseen: exploit information hidden in noise, BZ & GJC, Applied Intelligence (2022)

Concrete specification

✔	carbonation	< 2.34 mm $day^{-1/2}$
⬇	environmental impact	< 0.107 kg CO_2 e kg^{-1}
✔	cost	< 0.028 £ kg^{-1}
✔	density	< 2350 kg m^{-3}
✔	strength	> 20 MPa

Concrete design

10.5% cement

48.4% gravel

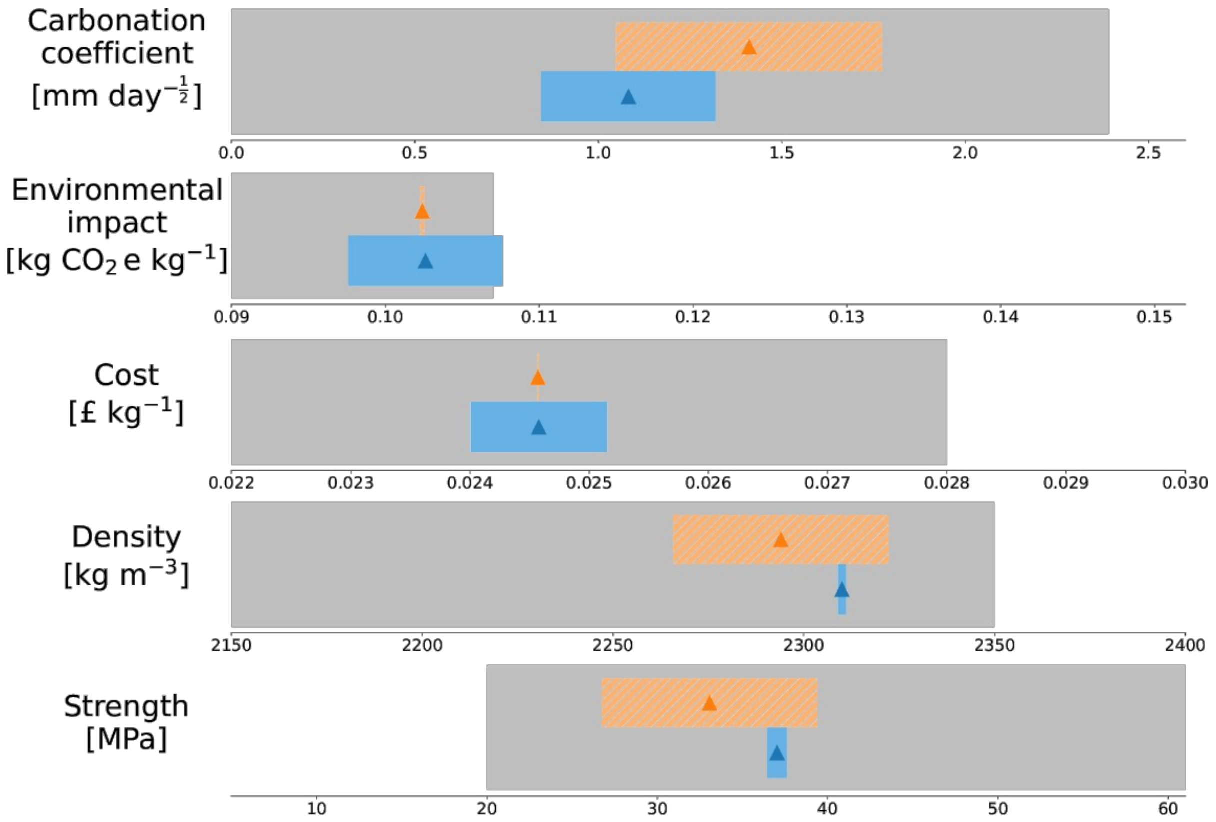
32.6% sand

8.5% water

Concrete manufacture

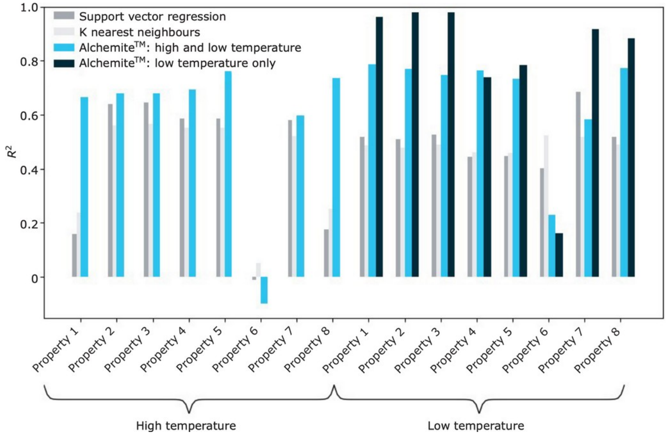
Probabilistic selection and design of concrete using machine learning
JCF, BZ, JML & GJC, Data-Centric Engineering **4**, e9 (2023)

Experimental validation of the proposed mixes

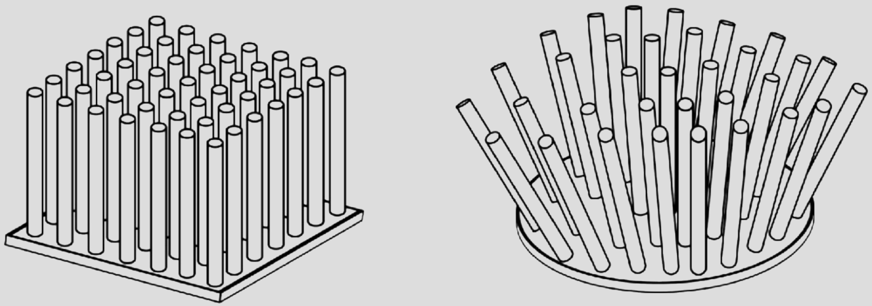


Model
Experiment
Target

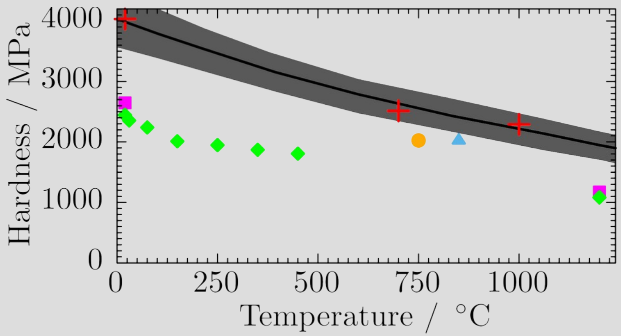
Probabilistic selection and design of concrete using machine learning
JCF, BZ, JML & GJC, Data-Centric Engineering **4**, e9 (2023)



Johnson Matthey Technology Review
66, 130 (2022)



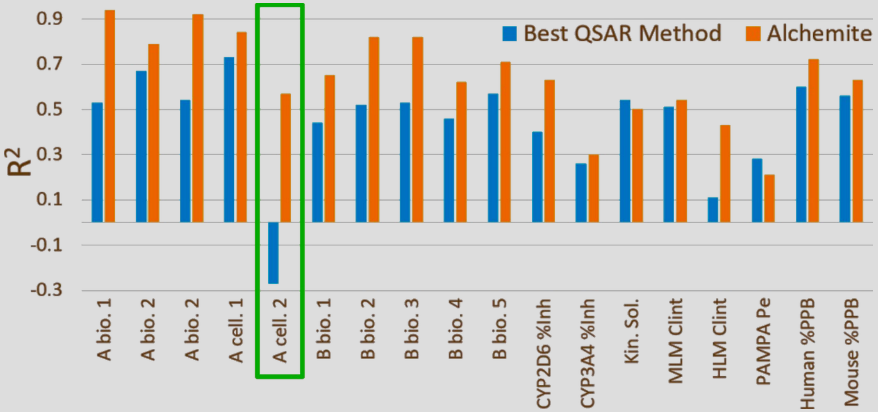
NASA Technical Memorandum
20220008637



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)

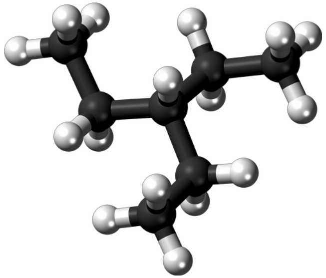


J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

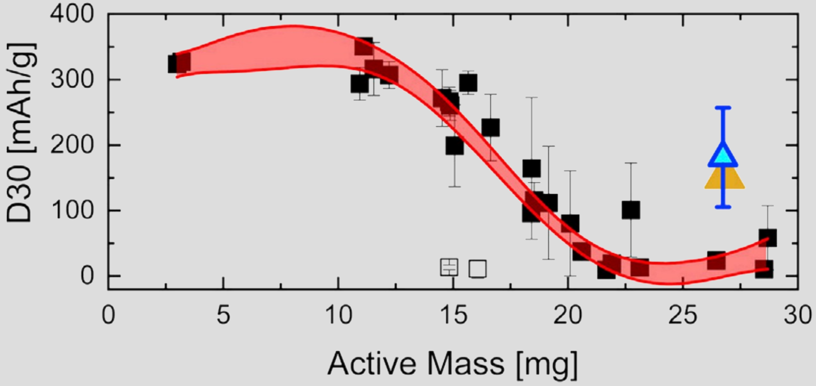
optibrium
iff

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)

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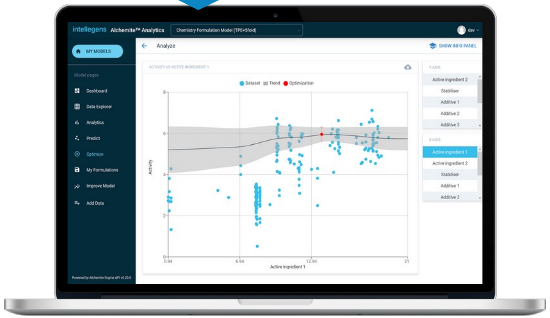
Fast start, easy-to-use, visual



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Lab systems

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Guide experiments, predict, design, optimize

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Integrate into your workflow (API, Python)

Advanced configuration, enterprise deployment

Alchemite™ Academic Programme

Access Alchemite™ for academic research

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

Designed and experimentally verified alloy for direct laser deposition

Exploited information in noise to design experimentally verified concrete

Software product taken to market through startup Intellegens