UNIVERSITY OF CAMBRIDGE

Modern-day blacksmith

Gareth Conduit

Machine learning for engineering faces the challenge that

not everything has been measured so data is sparse

Actively pursue two approaches to empower machine learning

not everything has been measured so data is **sparse**

Exploit **property-property** relationships to **merge** data, simulations, and physical laws

Adaptive **design of experiments** to accelerate discovery

Black box machine learning for materials design

Composition

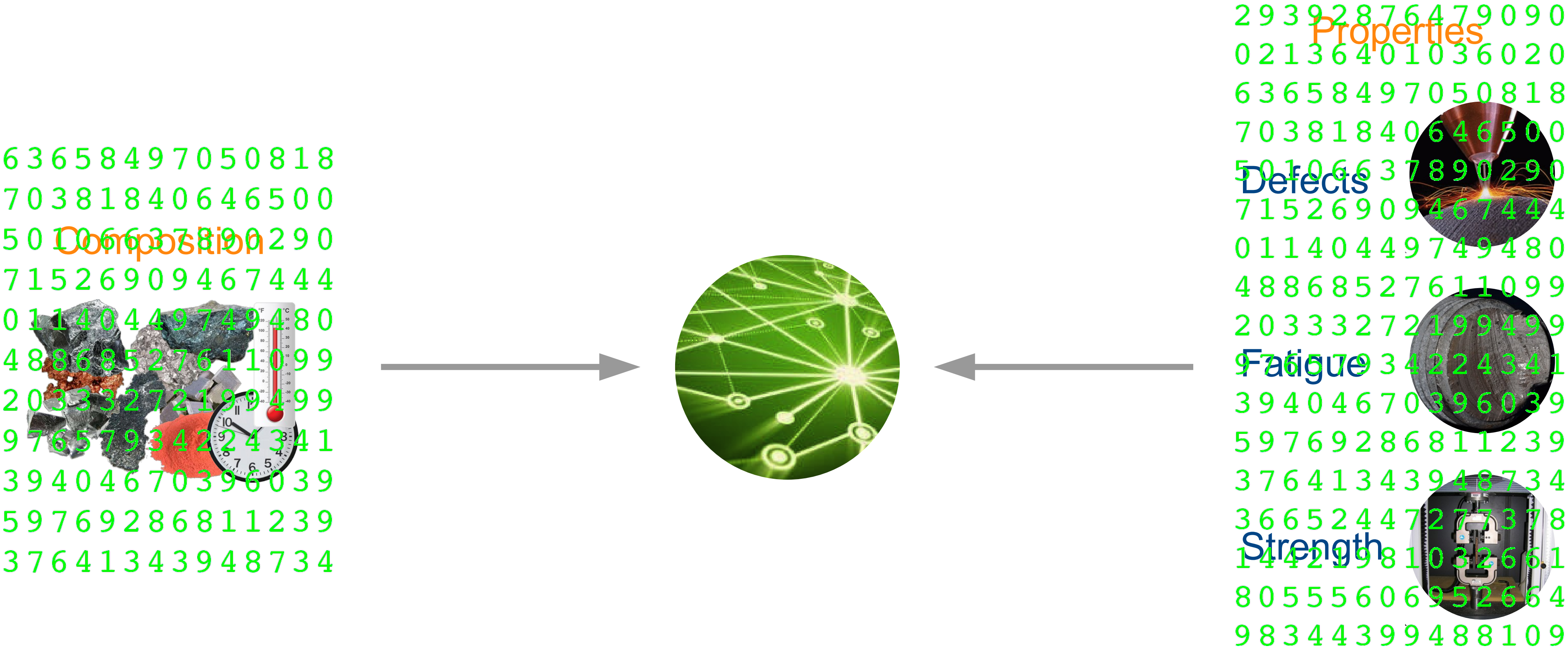
Properties

Defects

Fatigue

Strength

Train the machine learning



Machine learning predicts material properties

Composition

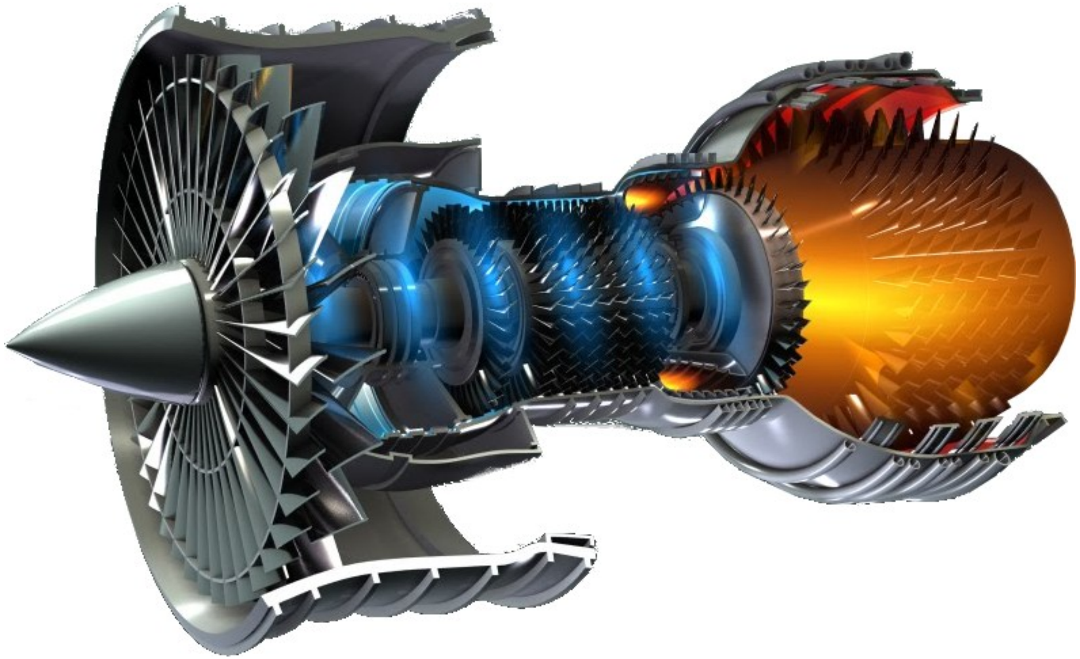
Properties

Defects

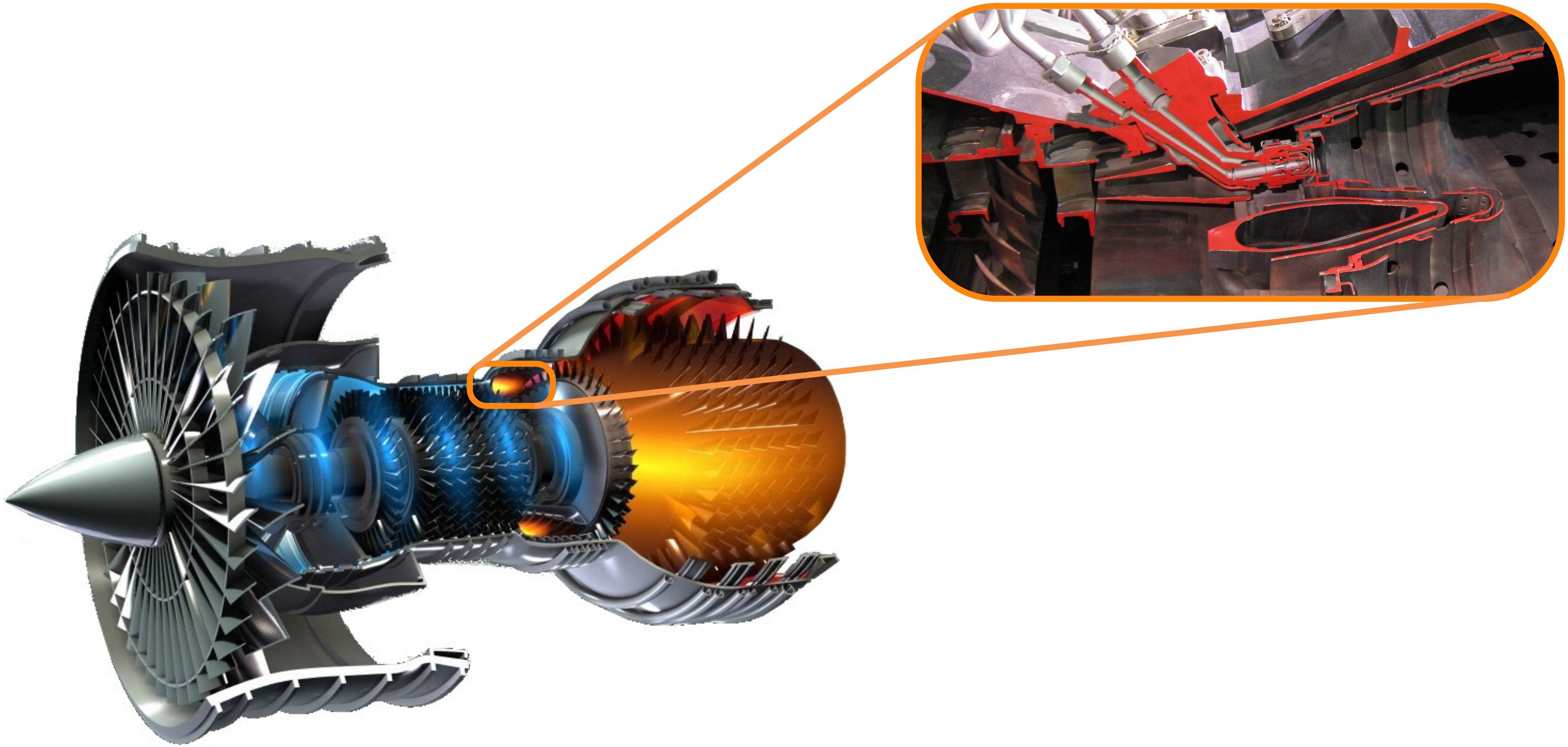
Fatigue

Strength

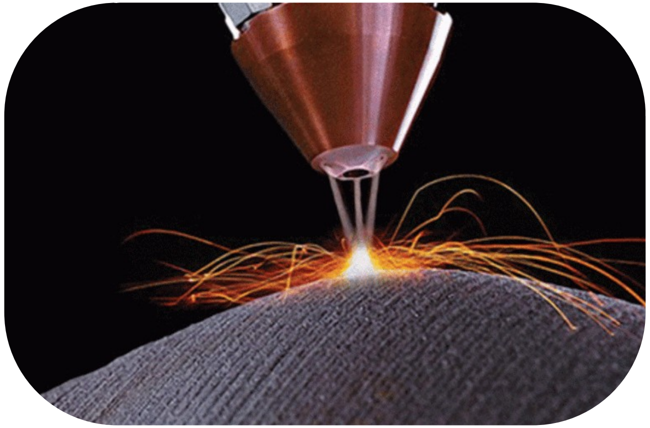
Jet engine schematic



Combustor in a jet engine



Direct laser deposition



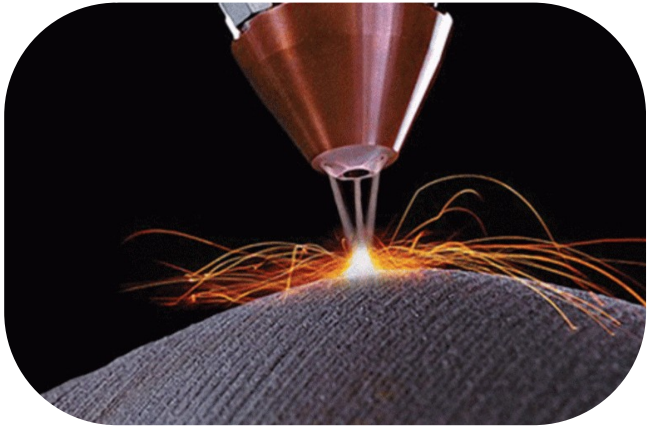
Data available to model defect density

Composition and heat treatment space 30 dimensions

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

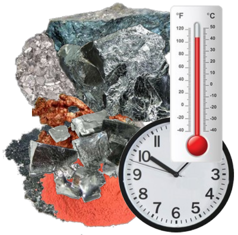
Ability for printing and welding are strongly correlated



Laser

Electricity

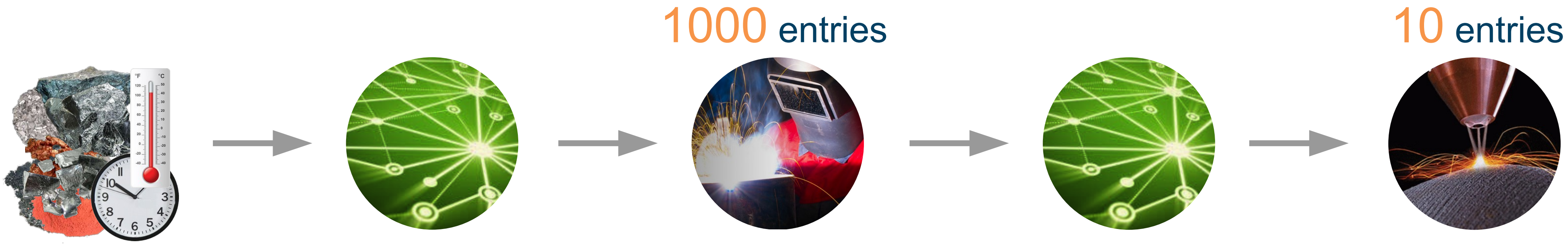
First predict weldability



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

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%

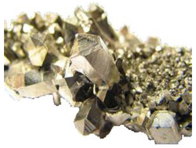
Co 4%

Mo 4.9%

W 1.2%

Zr 0.05%

Nb 3%



Al 2.9%

C 0.04%

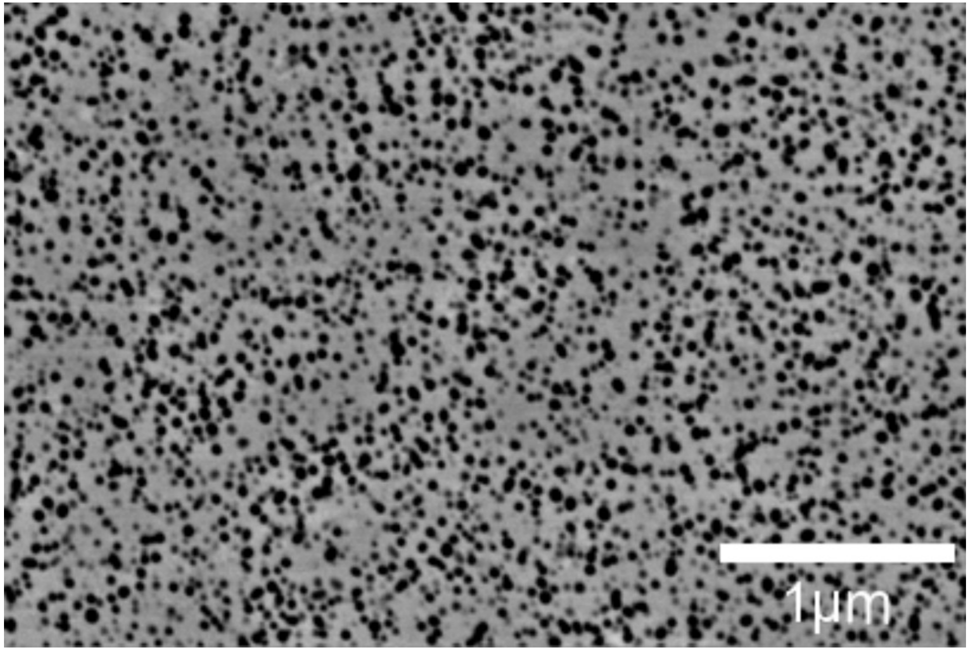
B 0.01%

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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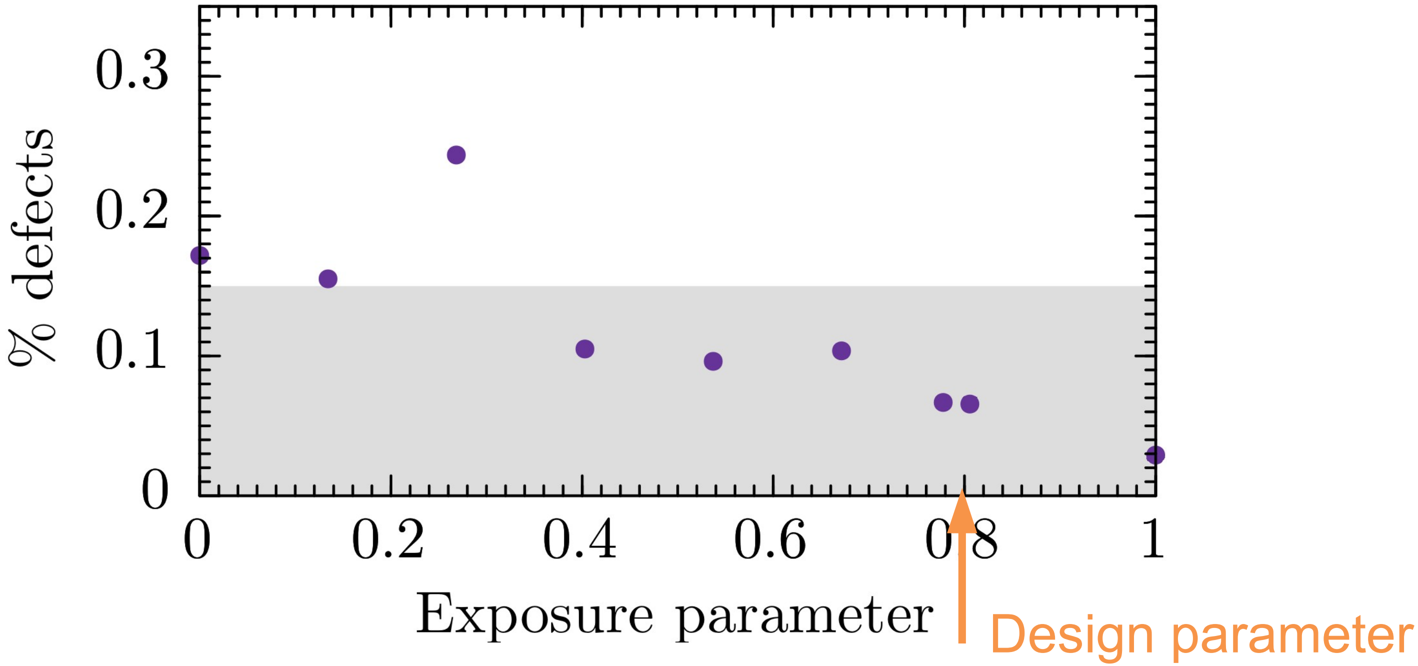
Testing the defect density



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Project MEDAL

Commissioning an
additive manufacturing machine
is time consuming

Propose process parameters for the
400W M2 from GE Additive
with the new additive-specific
Aheadd® CP1 powder from Constellium

The University Of Sheffield. AMRC Advanced Manufacturing Research Centre
BOEING
Constellium
GE Additive

How do you solve a problem like materials design?

Try every possible material

Guaranteed to find the best material

Many possibilities

Budgets / timescales

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Budgets / timescales

Ask an expert

Uses knowledge from past projects

Expensive resource

May retire or leave

Human after all!

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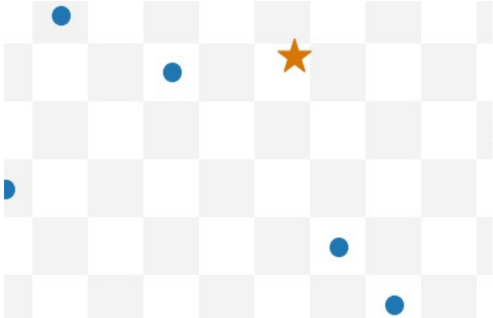
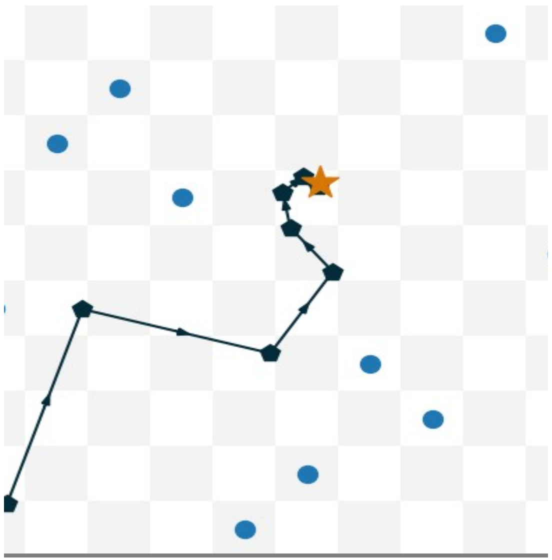


Structured design / DoE

Efficiently covers design space

Does not take advantage of accumulated knowledge

Machine learning approach



Machine learning-driven
adaptive experimental design

- ✓ Target-driven: actively search for successful materials
- ✓ Natively handle 100s or 1000s of variables
- ✓ Takes advantage of accumulated knowledge

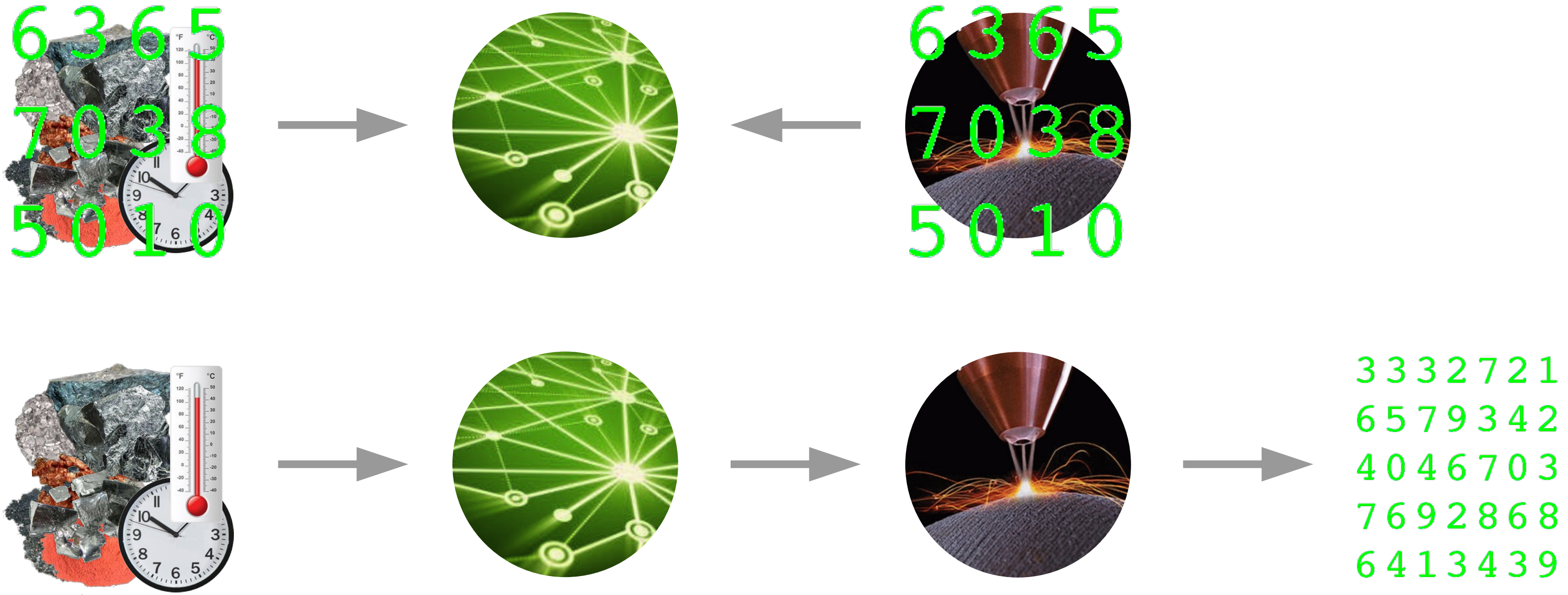
Train machine learning on initial data set

Train machine learning on initial data set

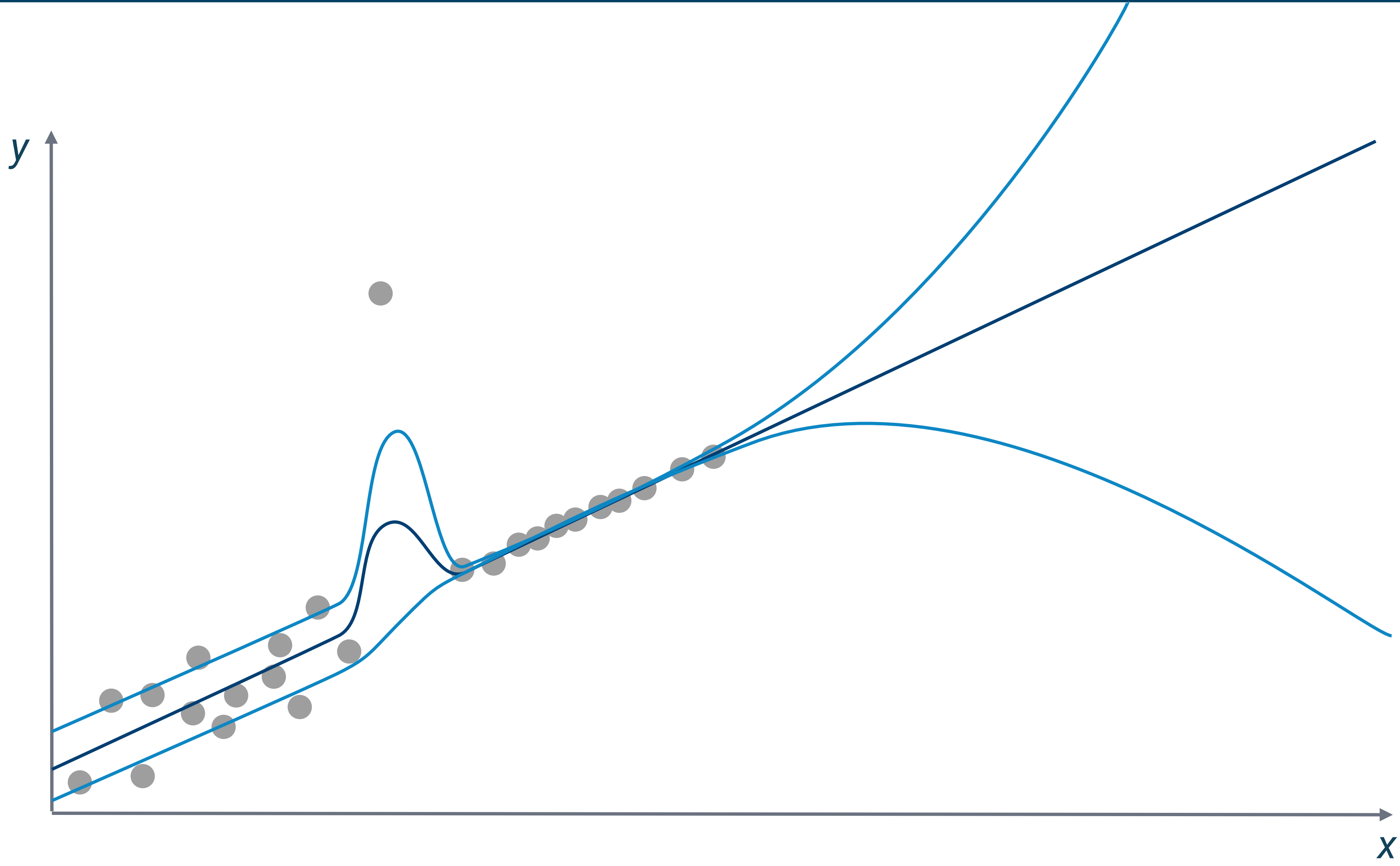
Machine learning proposes additional data to collect

Train machine learning on initial data set

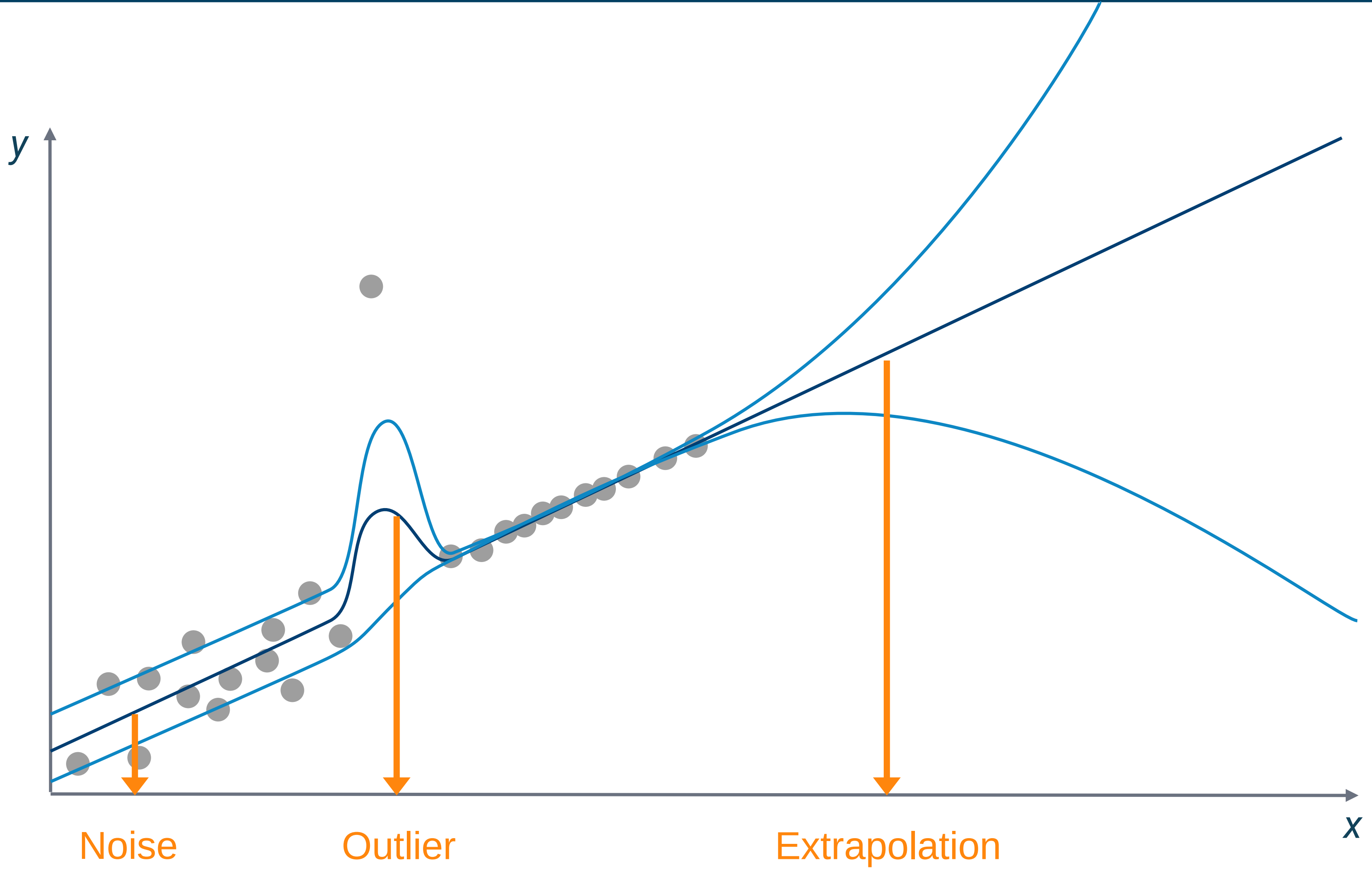
Machine learning proposes additional data to collect



Uncertainty estimated with machine learning



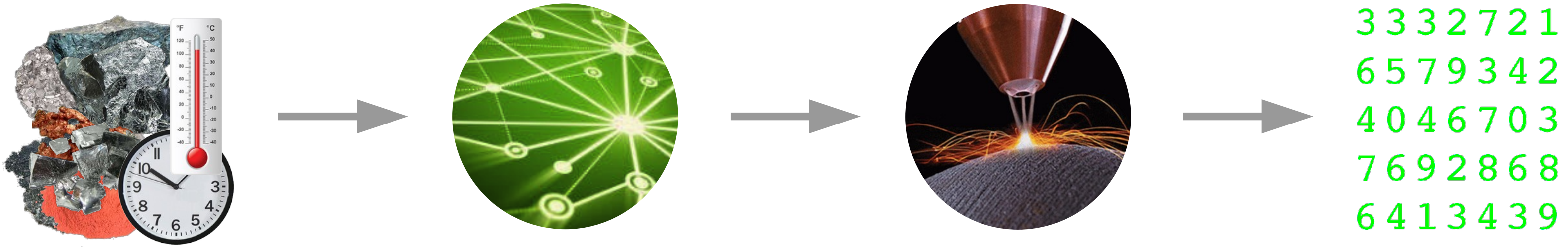
Interrogate machine learning of where to collect data



Train machine learning on larger data set

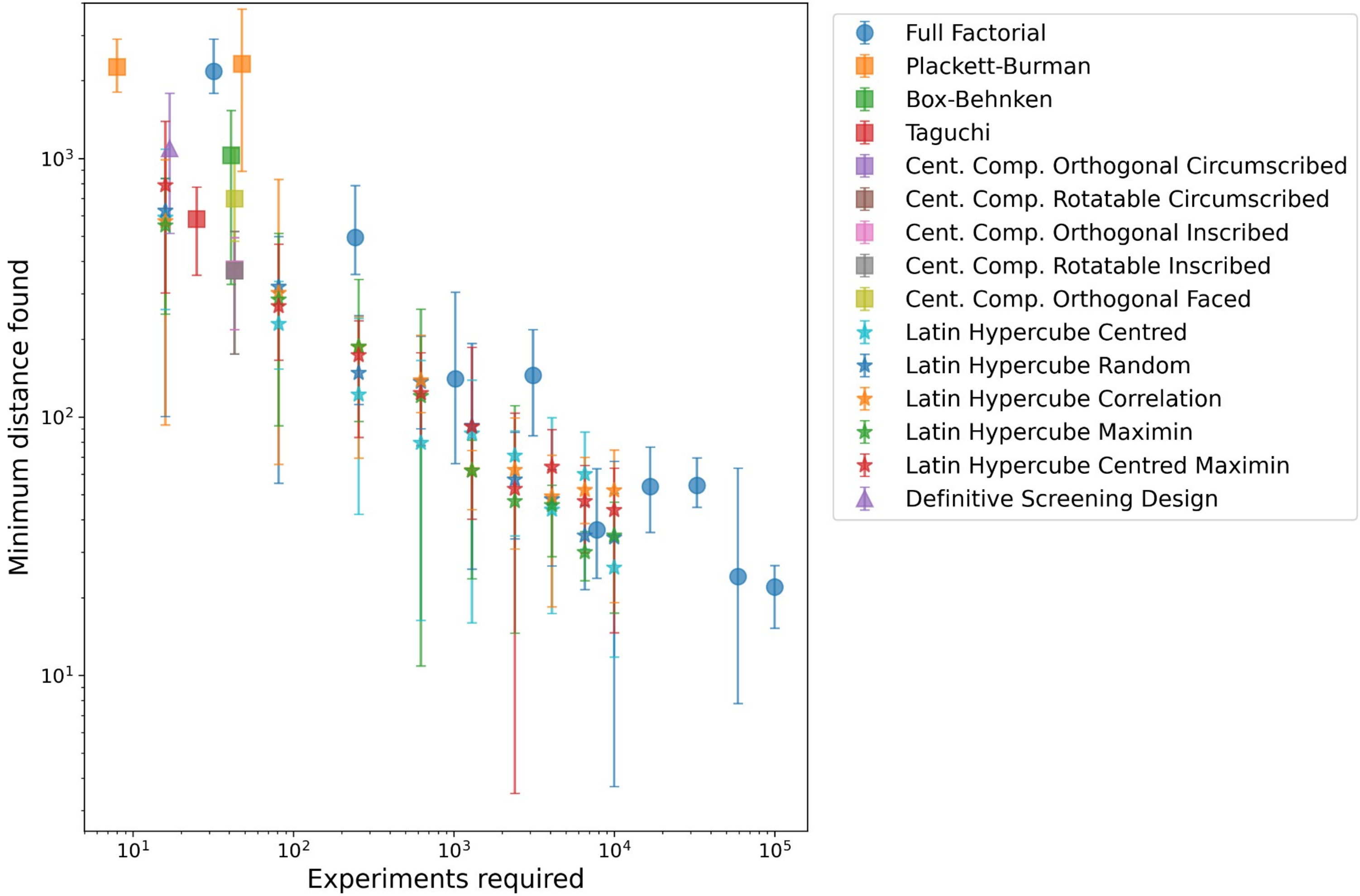
Train machine learning on initial data set

Machine learning proposes additional data to collect

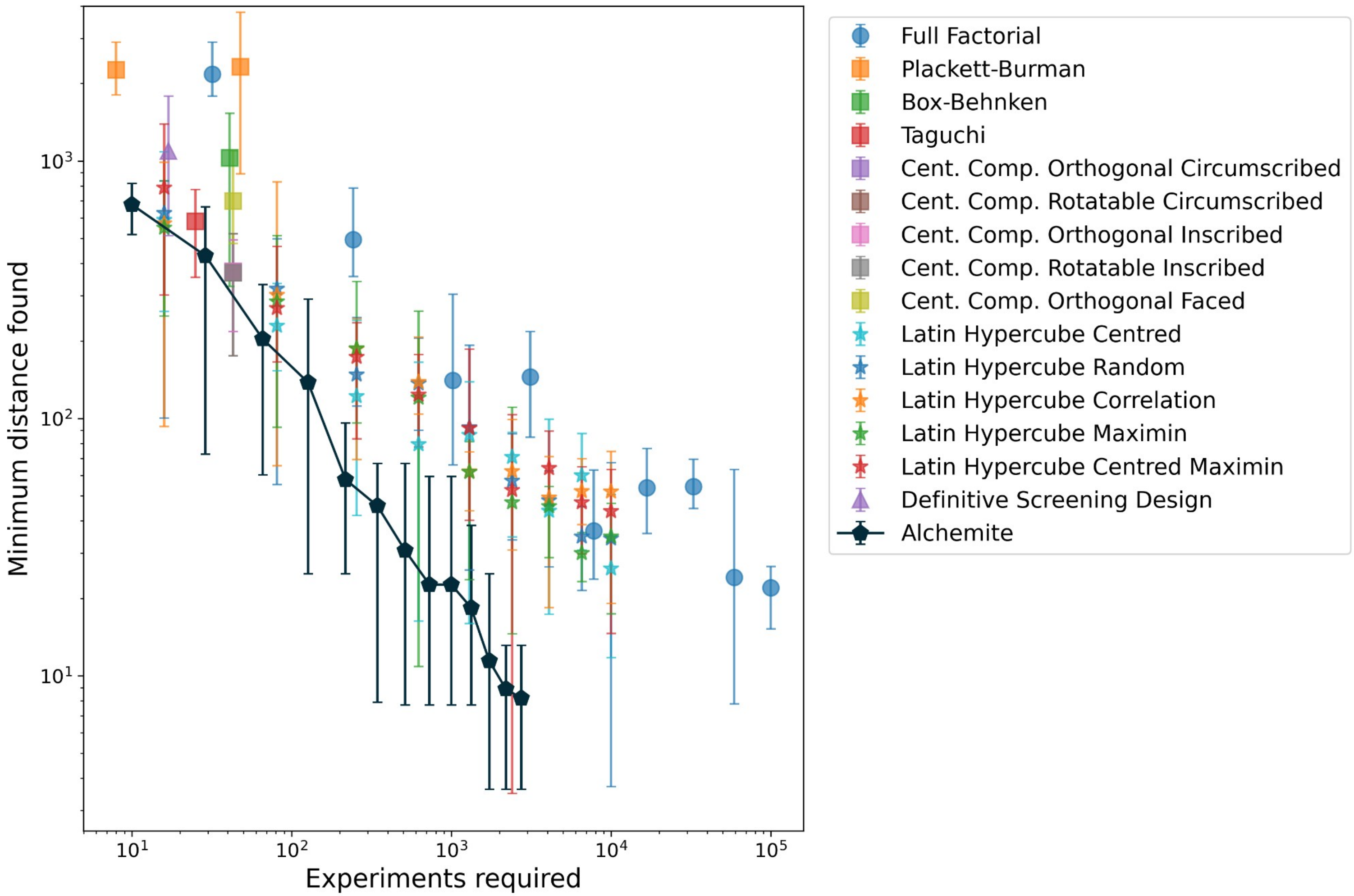


Train machine learning on larger data set

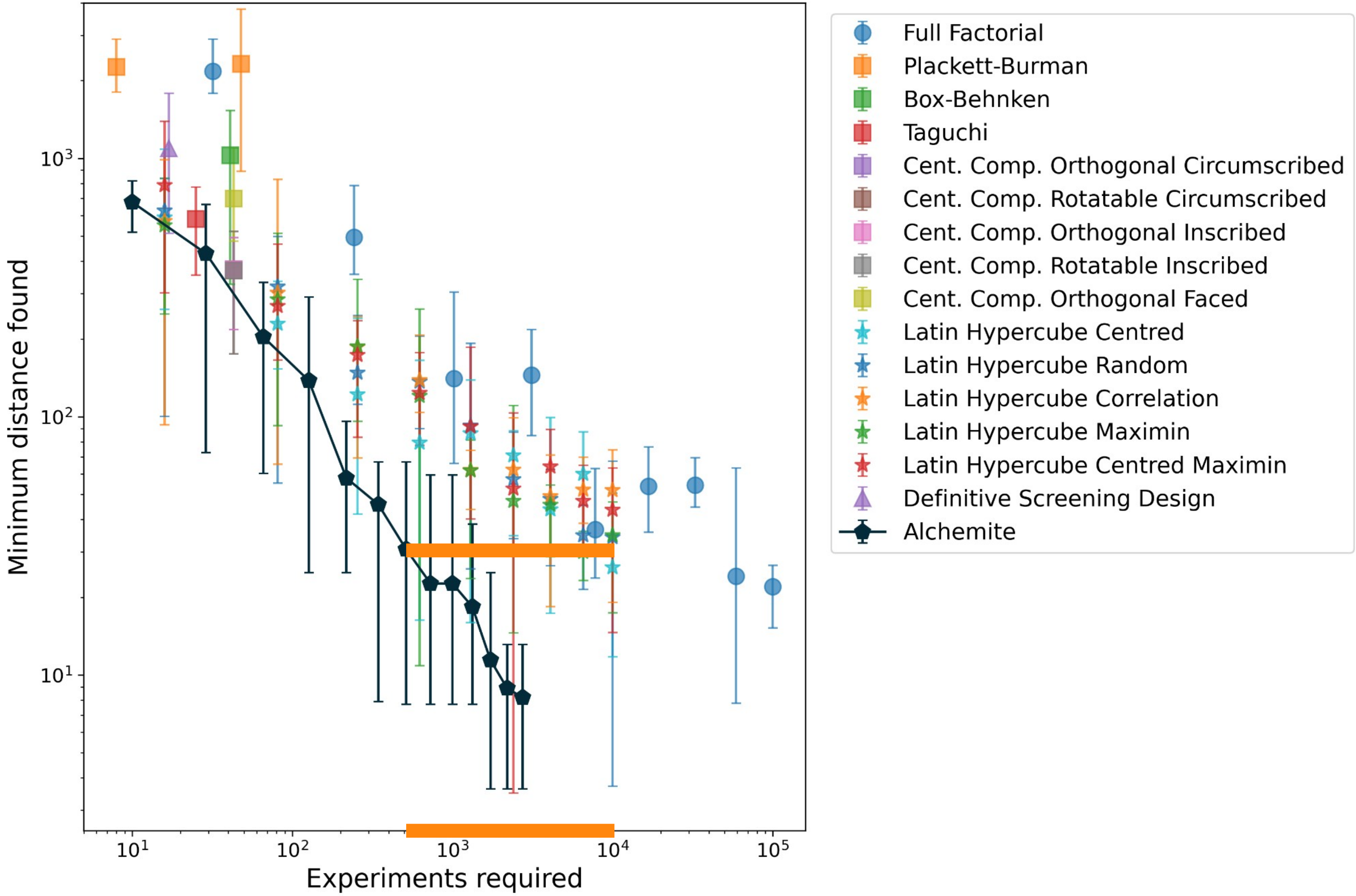
Structured experimental design



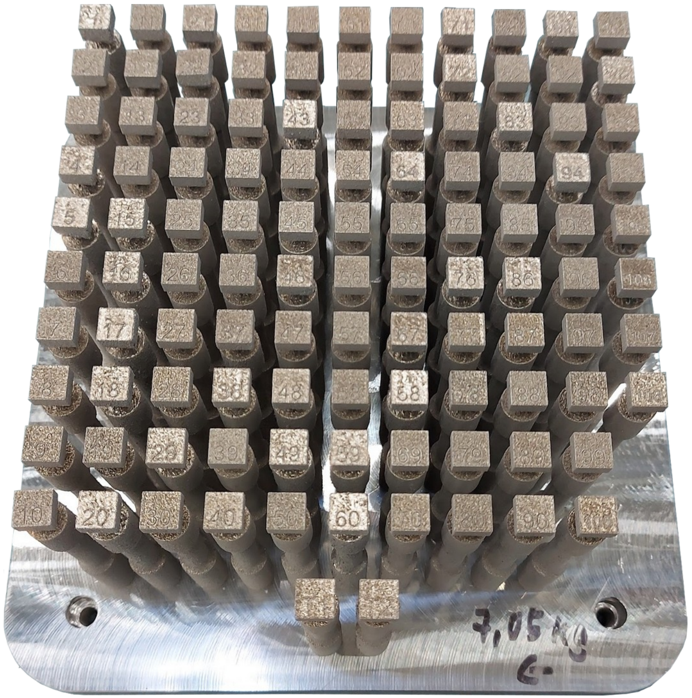
Adaptive experimental design

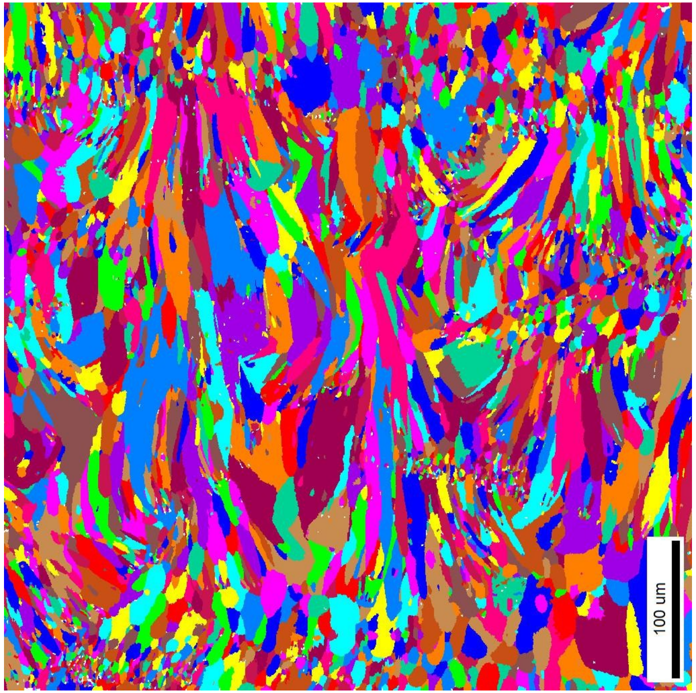


Adaptive experimental design accelerates ×10

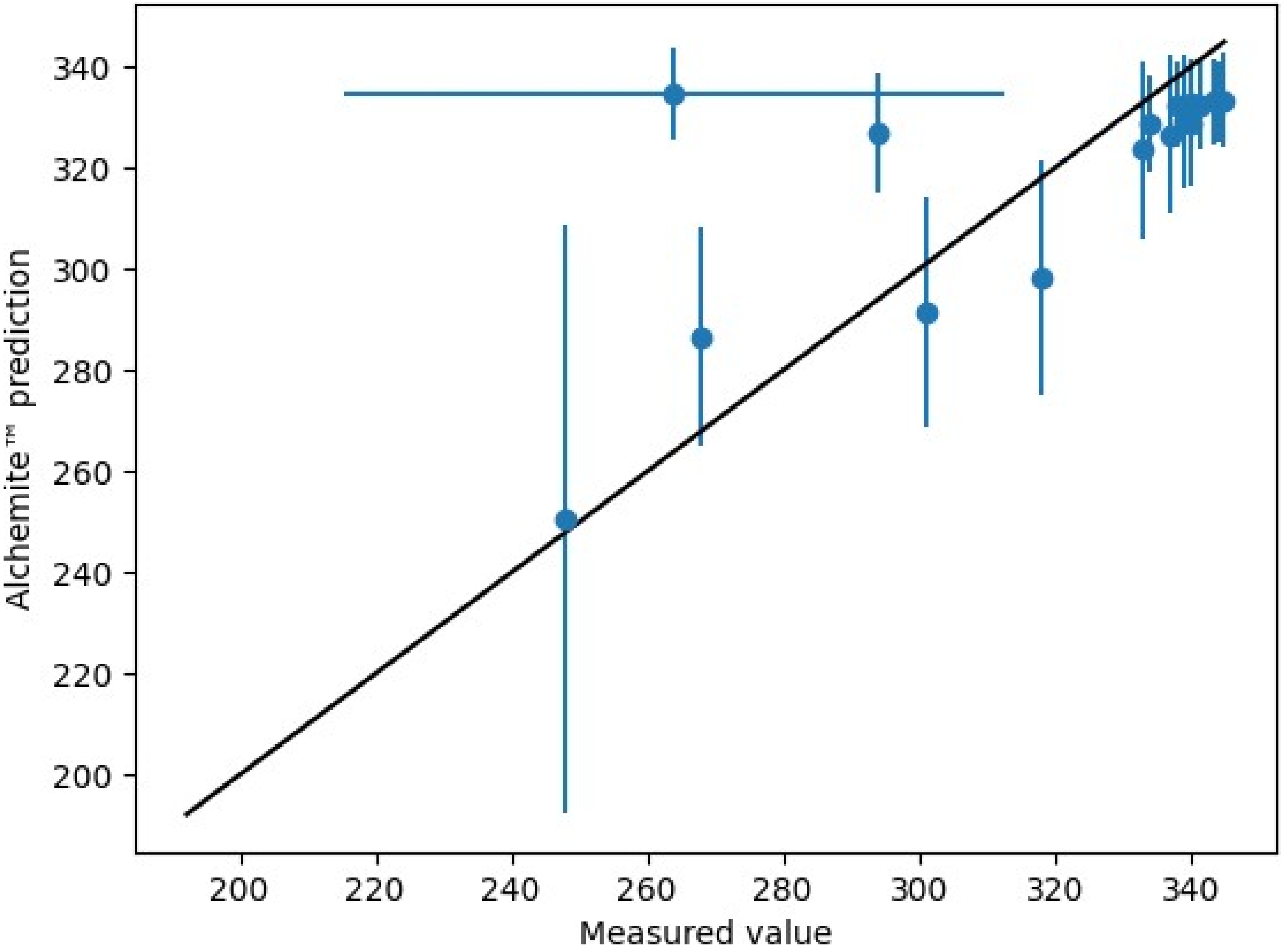


Project MEDAL proposed samples

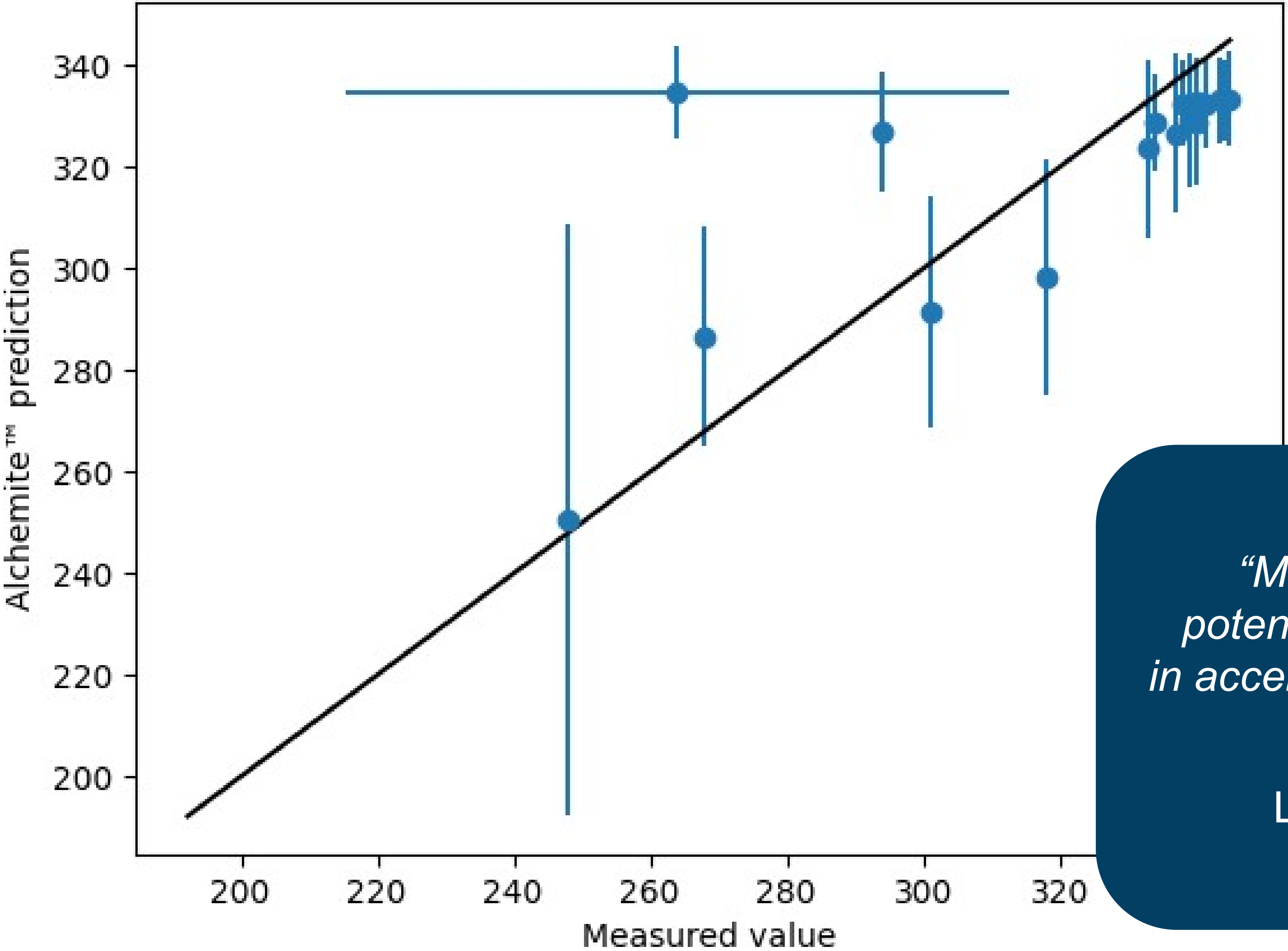




Project MEDAL model performance

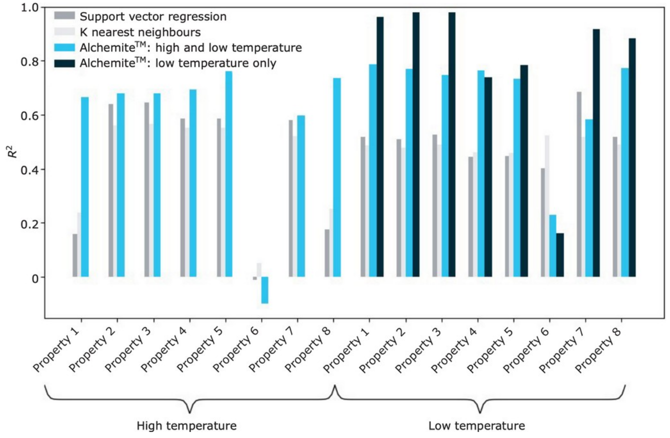


Project MEDAL outcome

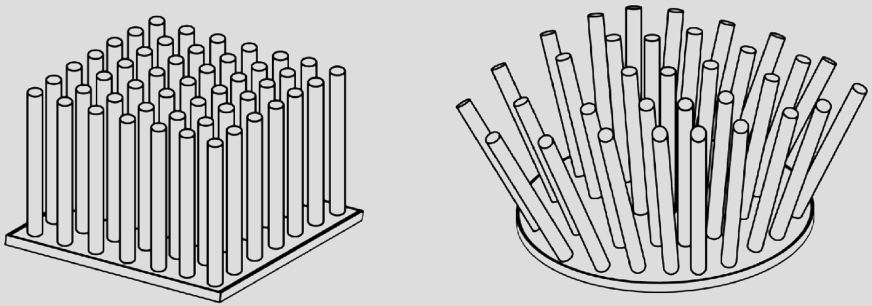


“Machine learning has the potential to be a key technology in accelerating further development and adoption of AM”

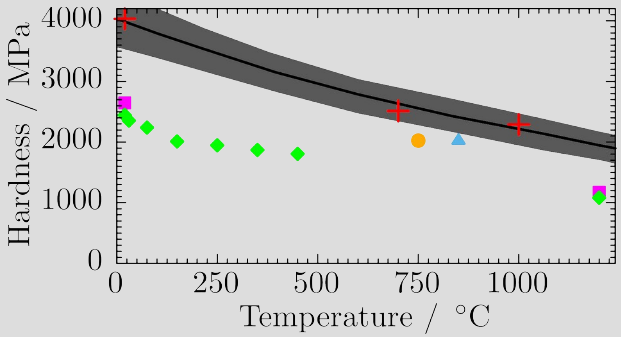
Lukas Jiranek, Boeing



Johnson Matthey Technology Review
66, 130 (2022)



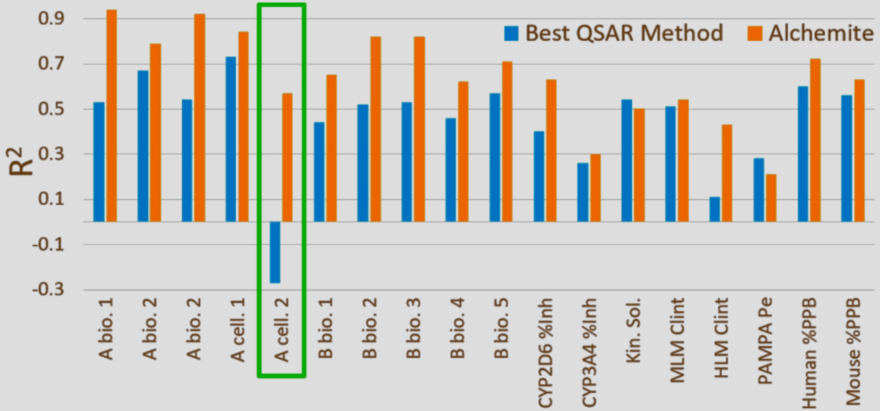
NASA Technical Memorandum
20220008637



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)



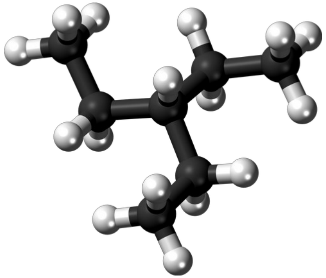
J. of Chem. Info. & Model. **60**, 2848 (2020)
Applied AI Letters **2**, e31 (2021)
Molecular Pharmaceutics **19**, 1488 (2022)

Constellation PHARMACEUTICALS
Takeda
AstraZeneca

optibrium™

iff

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



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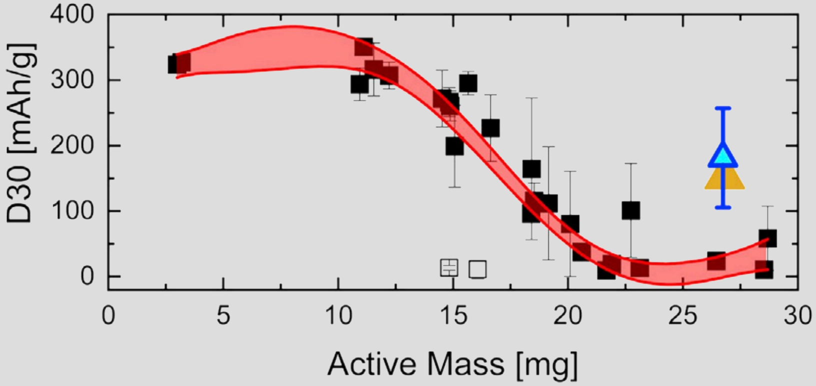
Fluid Phase Equilibria **501**, 112259 (2019)
Journal of Chemical Physics **153**, 014102 (2020)



Cell Reports Physical Science **2**, 100683 (2021)

UNIVERSITY OF BIRMINGHAM

Ansys
GRANTA

Summary

Exploit property-property relationships to improve predictions

Adaptive design of experiments accelerates discovery

Designed and experimentally verified alloys for direct laser deposition

Generic approach applied to alloys, batteries, pharmaceuticals, and beyond

Taken to market through Intellegens