UNIVERSITY OF CAMBRIDGE

intellegens

The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

Machine learning algorithm to

Train from sparse datasets

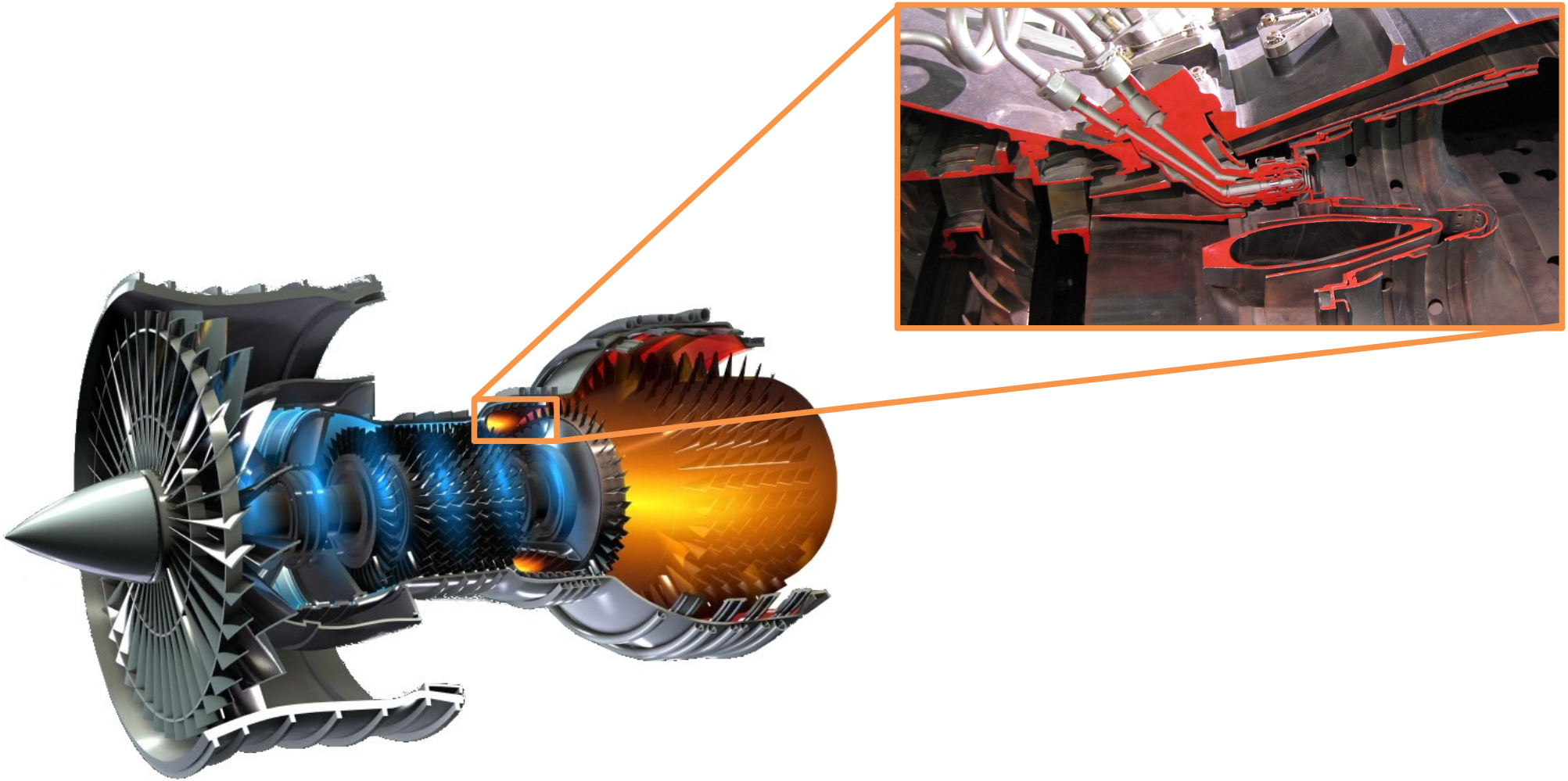
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

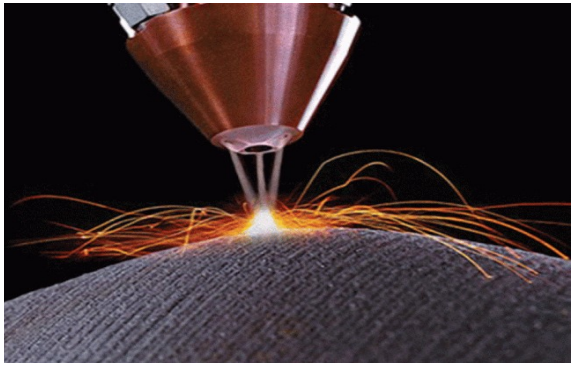
Accelerate discovery of new formulations

Generic with proven applications in materials and pharmaceuticals

Combustor for a jet engine

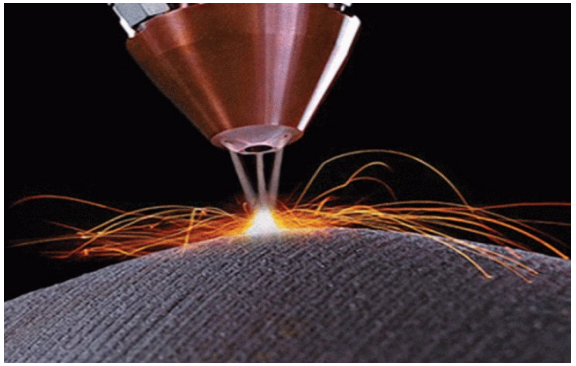


Direct laser deposition requires new alloys



Analogy between 3D printing and welding

Electricity



Laser

Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ' content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Processability	< 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

Cr: 19%

Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%

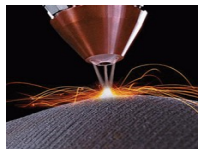
Al: 2.9%

C: 0.04%

B: 0.01%

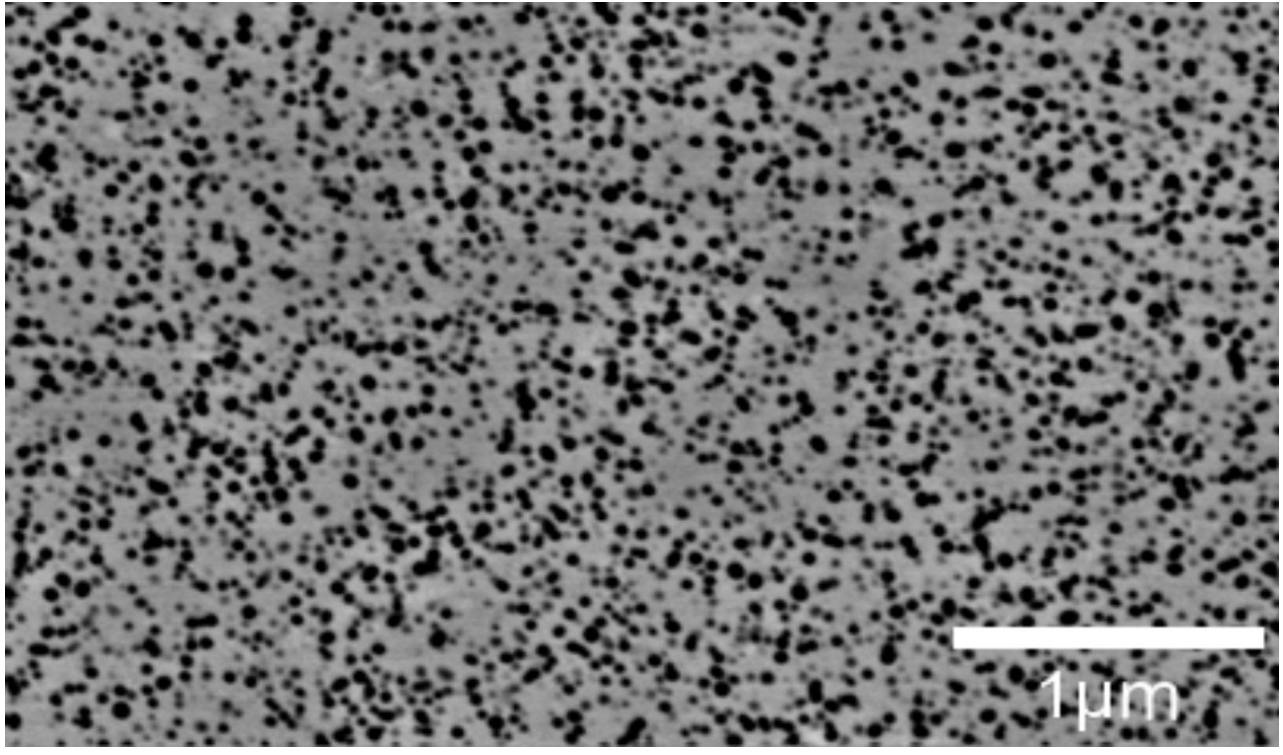
Ni

Expose 0.8

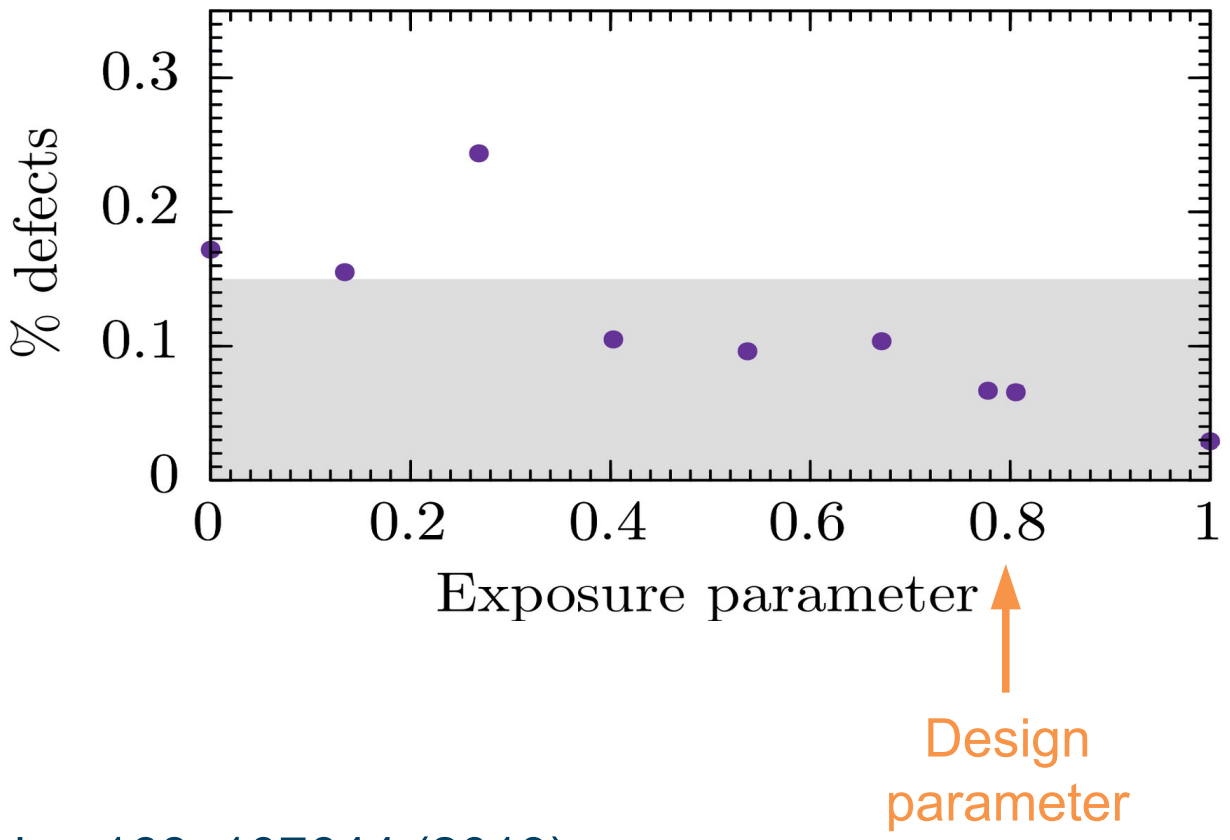


T_{HT} 1300ºC

Microstructure



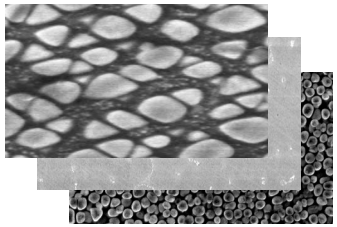
Testing the processability: horizontal printing



Materials & Design 168, 107644 (2019)

More materials designed

Nickel and molybdenum

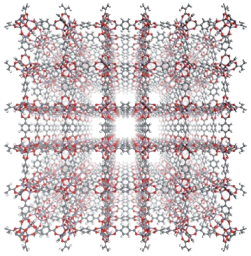


Steel for welding

Experiment and DFT for batteries

Application to chemicals and drugs

Metal organic framework



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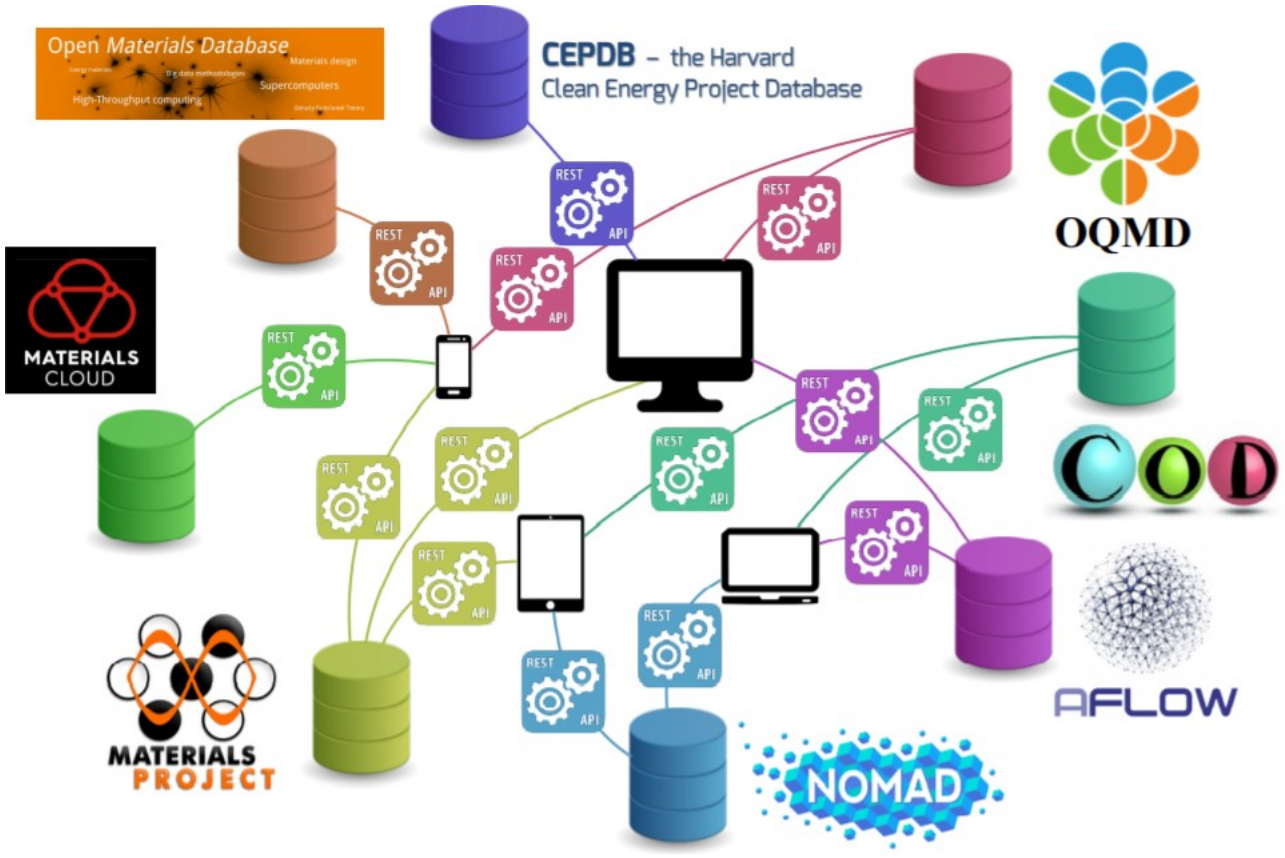
Lubricants with molecular dynamics and experiments

bp

Drug design

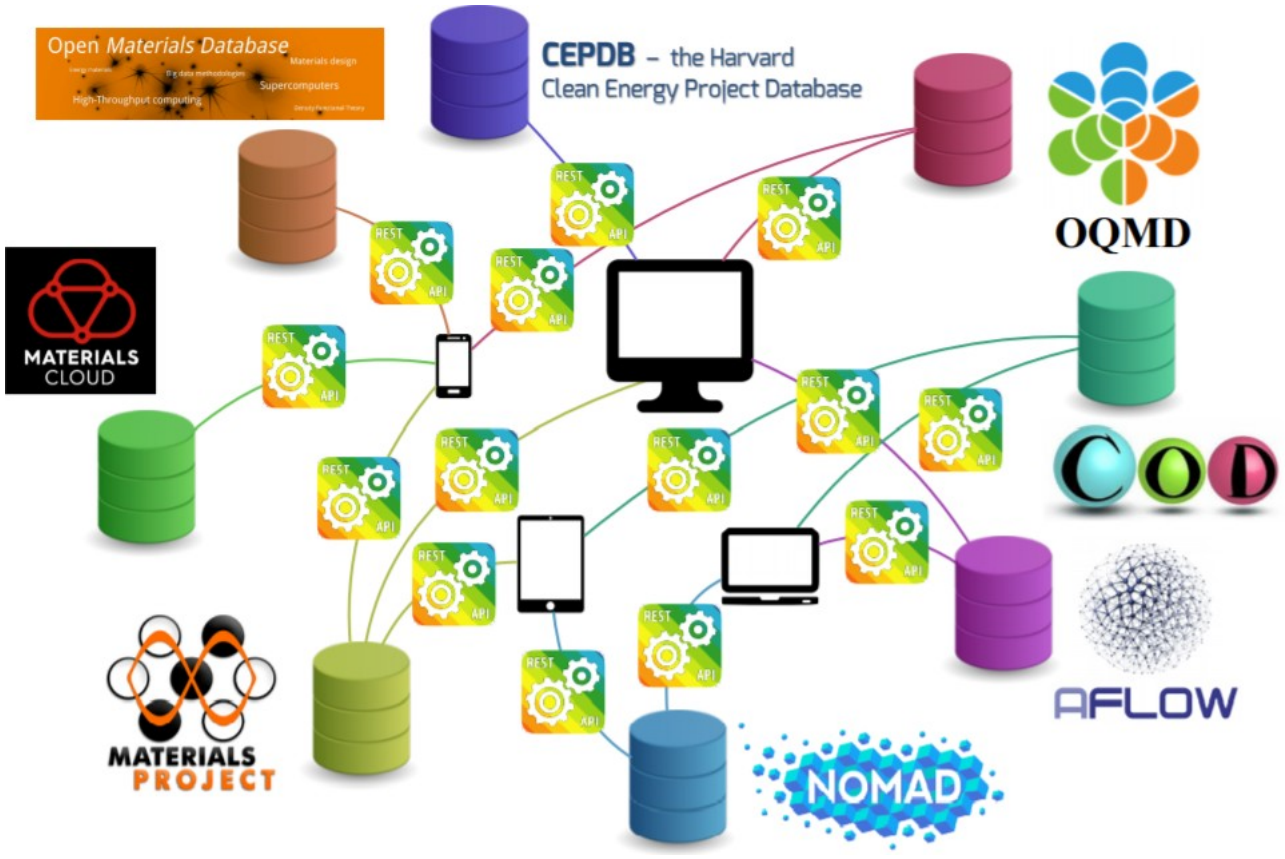
e-therapeutics
optibrium
AstraZeneca
Celgene
Takeda
Constellation
PHARMACEUTICALS

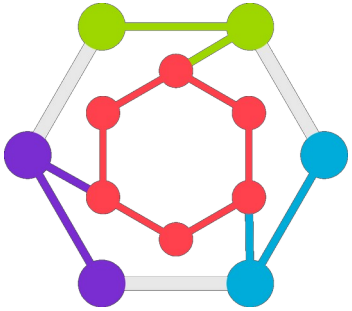
Machine learning requires extensive access to different databases



Each material database has a bespoke API, an obstacle for machine learning

OPTIMADE defines a common API





OPTIMADE provides a common API for accessing materials databases

www.optimade.org

Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Designed and experimentally verified alloy for direct laser deposition

Access databases through the OPTIMADE API

Marketed through startup intellegens, https://intellegens.ai/