Porous Metal Genomics for Tailoring Mechanical Properties of Light-weight 3D-Printed Architectures (PORMETALOMICS)

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Introduction

The

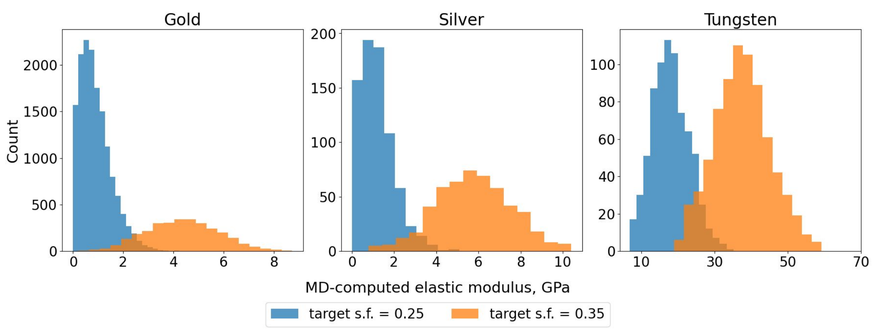
Porous metals, with pore sizes ranging from nanometers to millimeters, are increasingly important for emerging technologies due to their high surface-to-volume ratio and tunable mechanical properties. Applications include bone scaffolds, lightweight transport structures, and electrochemical electrodes. 3D printing enables the fabrication of complex porous architectures, but optimizing their mechanical properties remains challenging due to vast morphological variations.

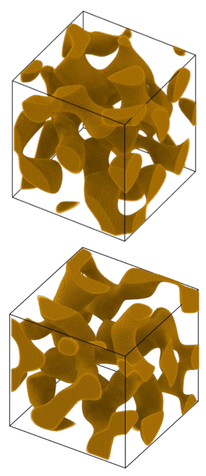
The **PORMETALOMICS** project develops methods to characterize porous structures, linking morphology to mechanical properties via geometrical and topological descriptors. Machine learning models predict mechanical behavior and guide the design of optimal structures using hierarchical screening and genetic algorithms. Experimental 3D printing validates these approaches, refining models and enabling the creation of tailor-designed materials for next-generation applications.

Developed tools

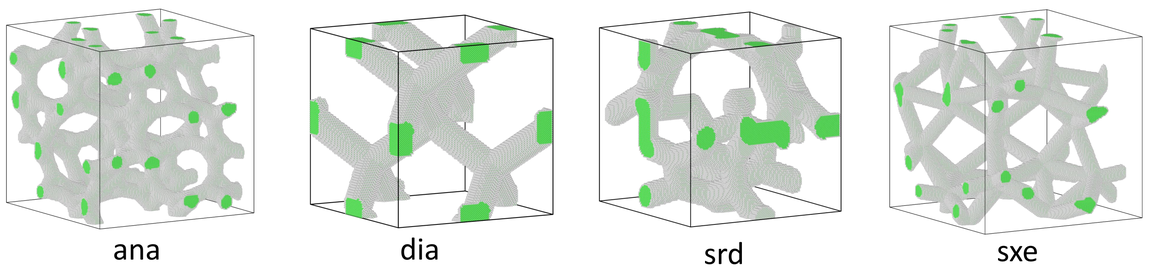
Porous structures generation:

- **Random structures from plane waves** - Dataset of 7000 structures, characterized with MD simulations (Au, Ag and W)





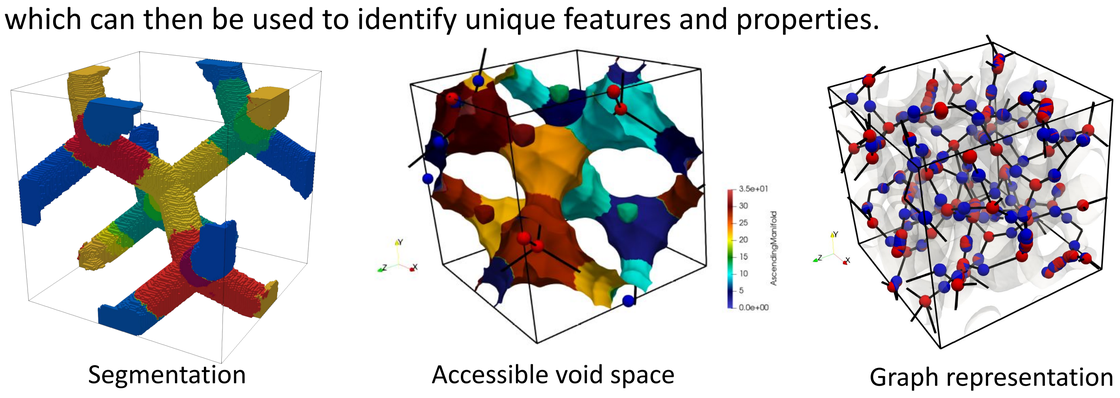
- Random structures from Voronois graphs
- **Architectured structures inspired by zeolites and Metal-Organic Frameworks** - dataset of 22 topologies with 5 values of solid fraction and 3 values of ligaments diameter.



- Spline method

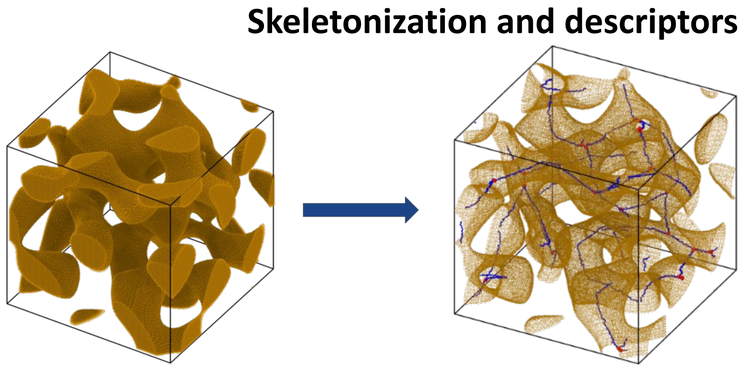
tda-segmentor*

Software package that segments a nanoporous material into different regions, which can then be used to identify unique features and properties.



* Vasudevan et al., Computer Physics Communications, 305:109344, 2024.

Skeletonization and descriptors calculation

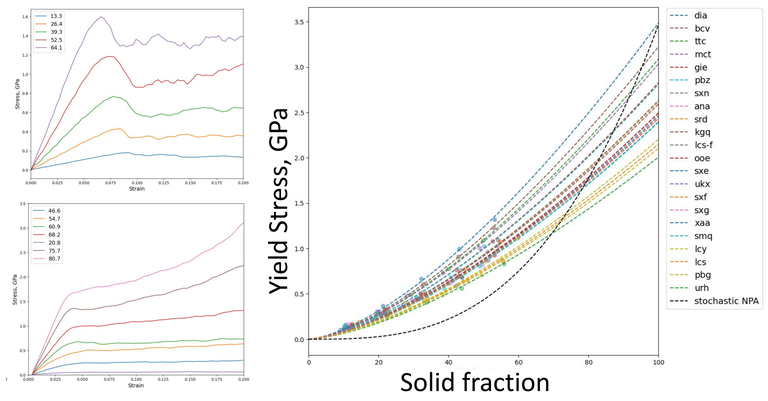


- Genus
- Number of nodes
- Nodes diameter
- Ligaments diameter
- Ligaments curvature

…

Results

A Molecular Dynamics Study of Chemistry-Inspired Nanoporous Aluminum Structures



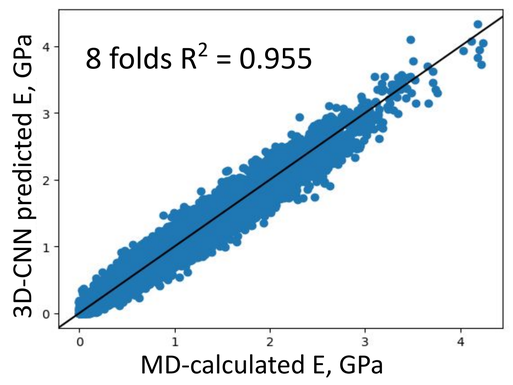
- Structures with defined topology were compared to stochastic NPA
- Each topology has different prefactors in the scaling laws:

$$\sigma = C_\sigma \rho^{1.5} \quad \text{(GPa)}$$

$$E = C_E \rho^{2} \quad \text{(GPa)}$$

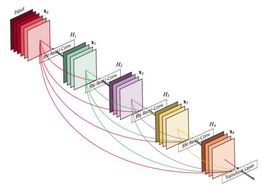
- Scaling laws remain constant at ligaments diameters of 7.5 and 10nm but might deviate at 5nm

Structure-property relationship in stochastic nanoporous metals with 3D Convolutional Neural Networks



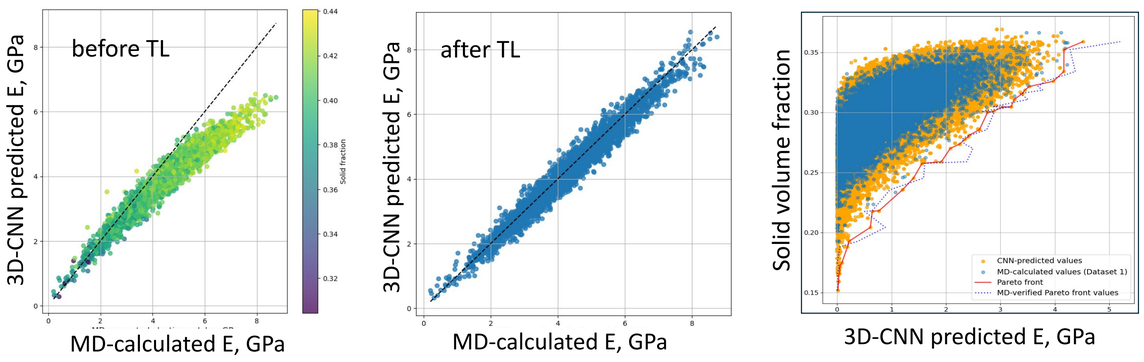
- Model trained on 5000 NPG structures tested in 3 directions - 15000 datapoints
- 3D-CNN architectures were compared to conventional descriptors-based approach
- DenseNet-121 demonstrated the best performance

LAMMPS



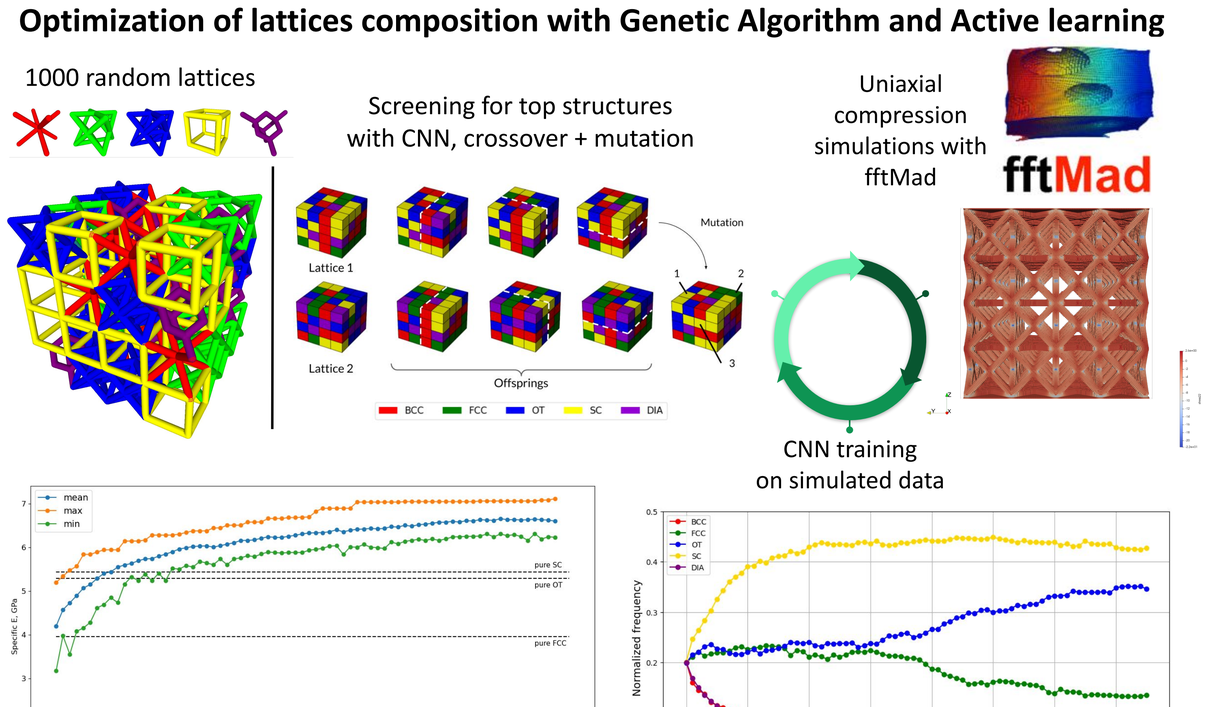
Transfer learning and search for best-performing structures

Base model trained on nanoporous gold structures with s.f = 0.25 was used to transfer knowledge to different materials (silver and tungsten) and different solid fraction (0.35)

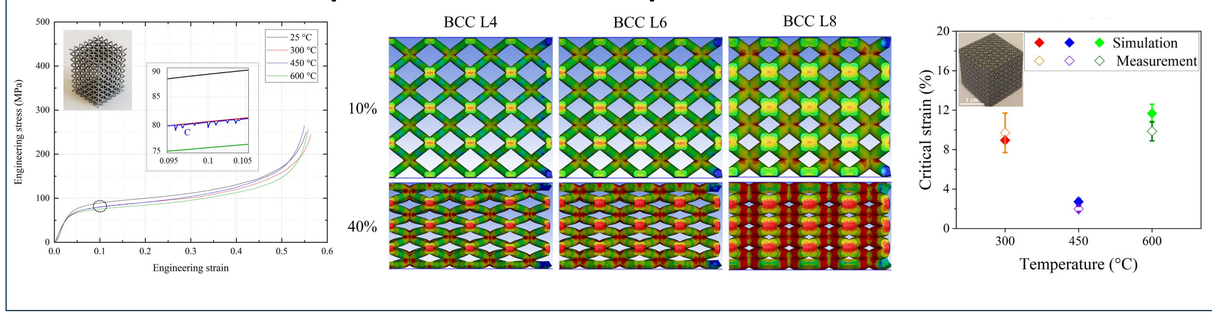


100.000 stochastic structures were estimated with trained model and Pareto front was verified with additional MD simulations

Optimization of lattices composition with Genetic Algorithm and Active learning



3D printed lattices and experimental validation



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