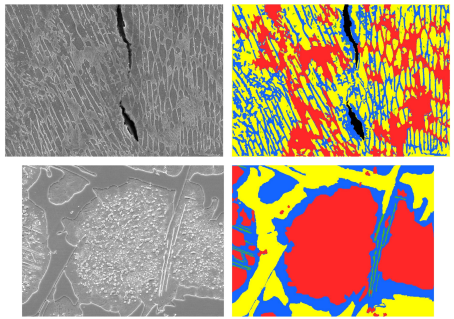
DIADEM Materials Grand Challenge 2025

Kick Off

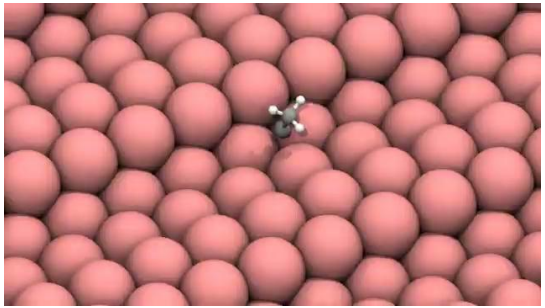
Challenges

Image Segmentation



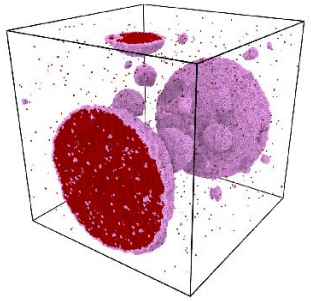
Develop **algorithms to precisely identify and delineate different phases** (e.g., grains, pores, inclusions) within microscopy images of metallic materials from the MetalDAM dataset, enabling quantitative analysis of microstructural features.

Interaction Potentials



Train **machine learning models to predict the interaction energy and forces** between atoms in catalytic materials using data from the Open Catalysis Project, ultimately aiming to accelerate the discovery of more efficient catalysts.

Generative Modelling

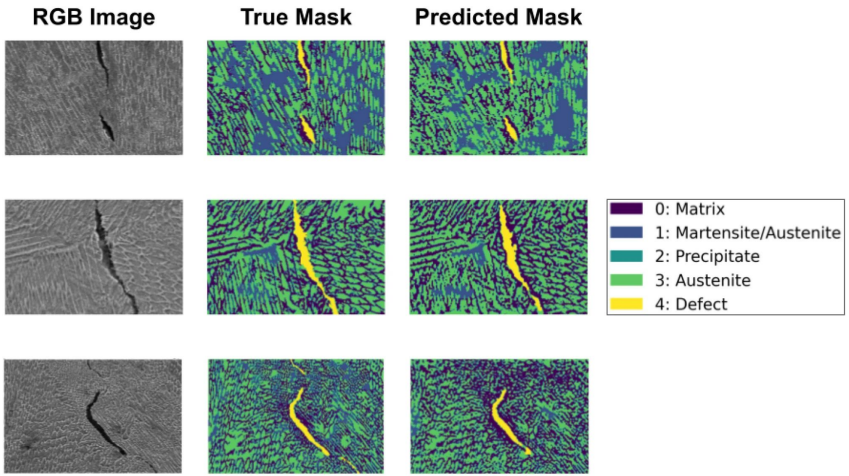


Students will leverage **generative modelling techniques to create realistic local atomic structures** of Tantalum, replicating the patterns observed during the initial stages of crystal nucleation as identified through topological analysis in the provided research.

Image Segmentation

Metallography Dataset from Additive Manufacturing (MetalDAM) dataset.

Gray scale images taken from scanning electron microscope (SEM):



The challenge

Devise an algorithm to classify each pixel into one of 5 categories by training on pre-labelled images.

Luengo, Julian, et al. "A tutorial on the segmentation of metallographic images: Taxonomy, new MetalDAM dataset, deep learning-based ensemble model, experimental analysis and challenges." *Information Fusion* 78 (2022): 232-253.
Biswas, M., Pramanik, R., Sen, S. *et al.* Microstructural segmentation using a union of attention guided U-Net models with different color transformed images. *Sci Rep* **13**, 5737 (2023). https://doi.org/10.1038/s41598-023-32318-9

Image Segmentation

42 - labelled images
164 - unlabelled

Task 1: (Supervised) train on a subset of the labelled image and test on the remainder.

Task 2: (Unsupervised) train on unlabelled images and test on labelled.

Luengo, Julian, et al. "A tutorial on the segmentation of metallographic images: Taxonomy, new MetalDAM dataset, deep learning-based ensemble model, experimental analysis and challenges." *Information Fusion* 78 (2022): 232-253.
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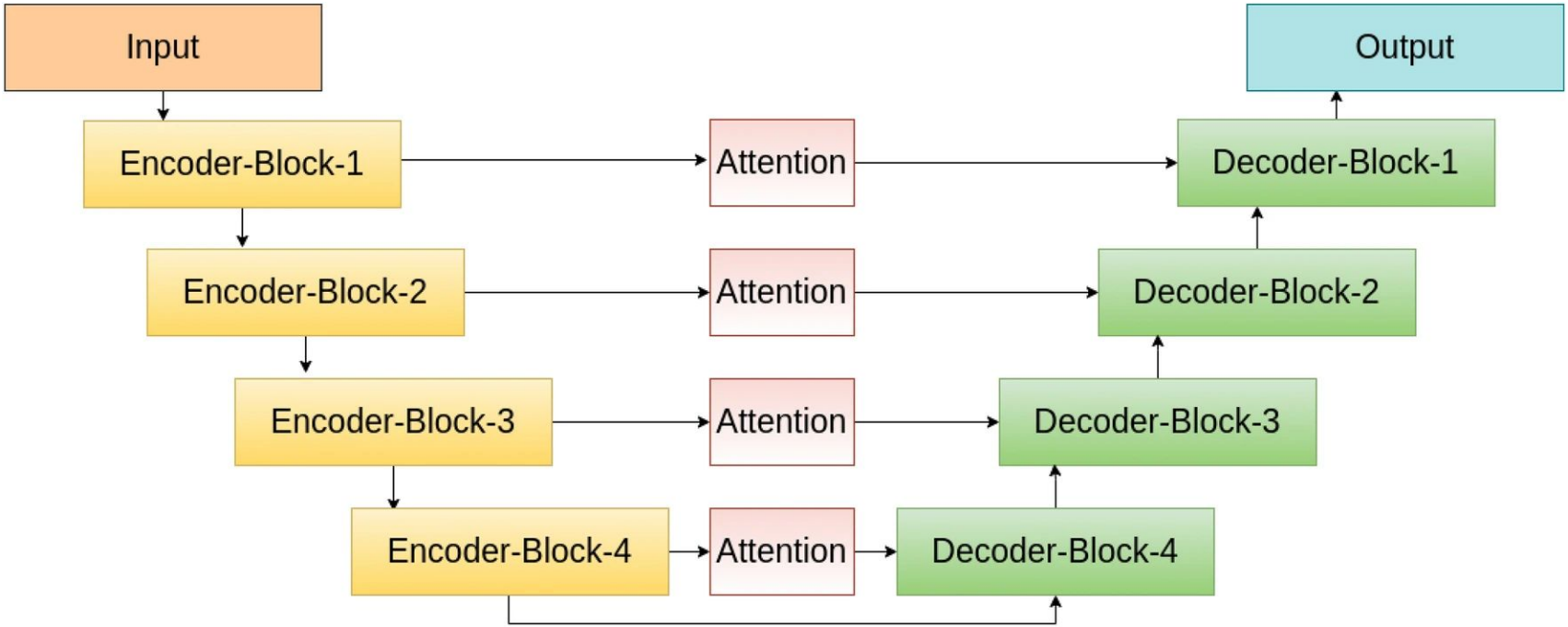
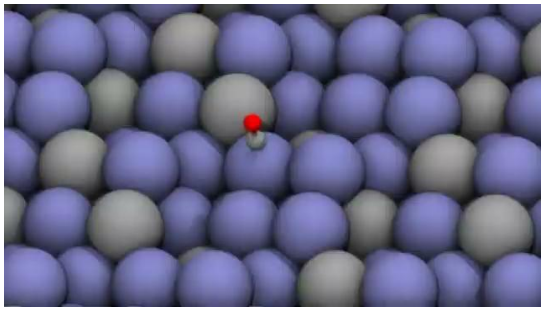
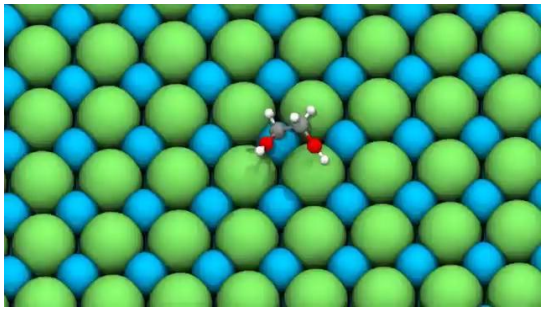
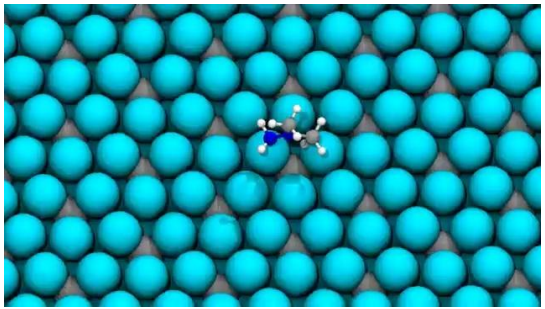
Image Segmentation



Interaction Potentials - Open Catalysis OC22

OC22 contains density functional theory (DFT) calculations of **atomic structures, energies, and forces for catalytic surfaces with adsorbates.** It provides large-scale data for training and benchmarking machine learning models aimed at predicting adsorption and reaction energetics across diverse catalyst compositions and surface geometries.

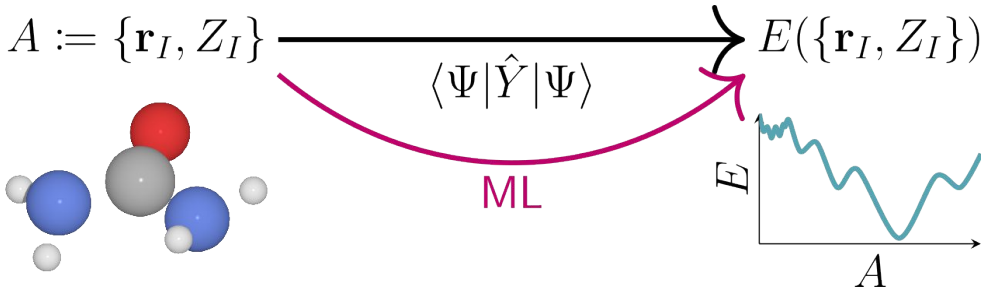




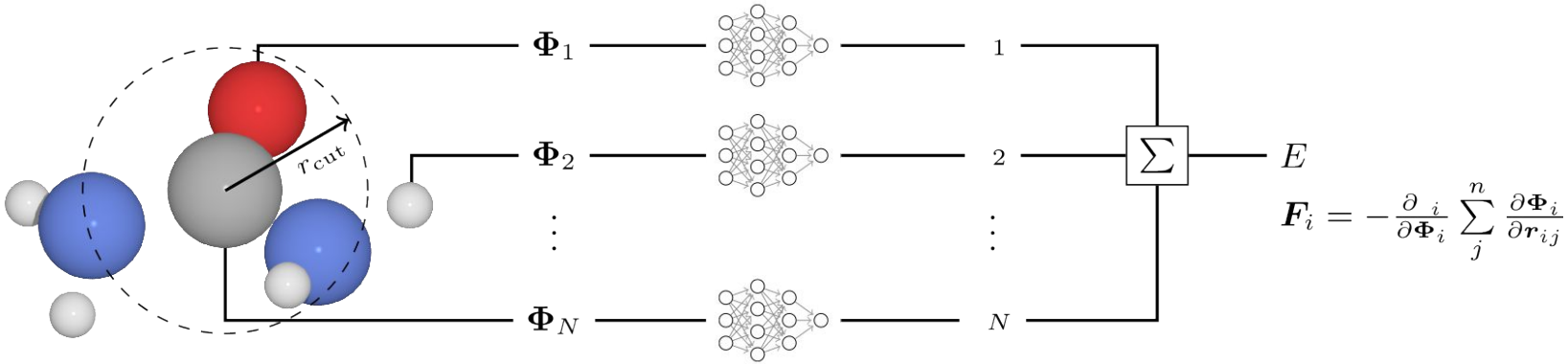
Interaction Potentials - Open Catalysis OC22

Task 1: Structure to Total Energy and Forces (S2EF-Total) task - lowest RMSE between your predictions and the DFT result.

Task 2: Initial Structure to Relaxed Structure (IS2RS) - starting with an unrelaxed structure, predict the geometry of the relaxed structure.

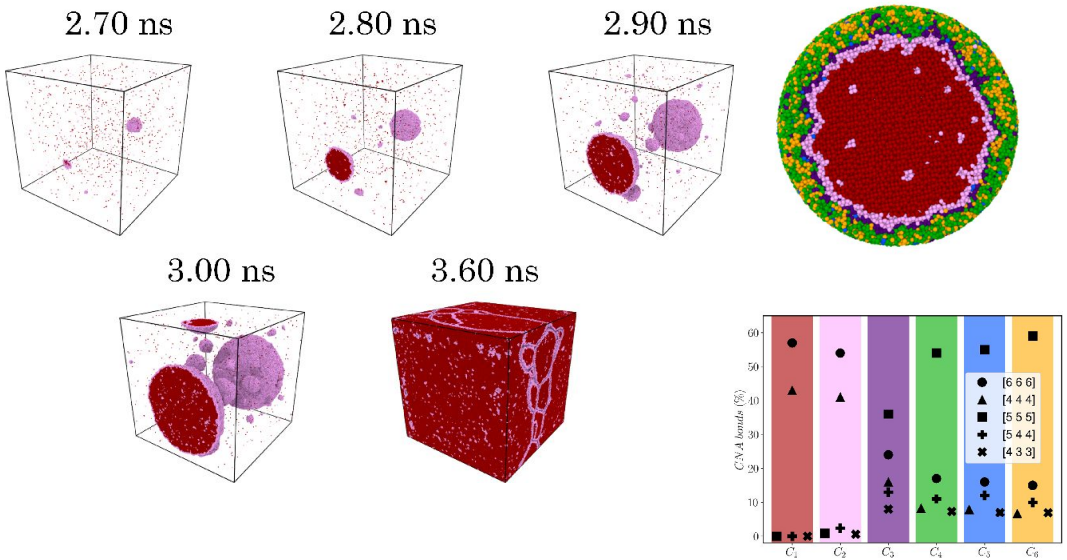
Interaction Potentials - Open Catalysis OC22





Generative Modelling - Solidification

Solidification of tantalum from ab initio molecular dynamics



The challenge

Devise an algorithm to generate atomic configurations that are statistically similar to those in the MD trajectory.

Becker, S., Devijver, E., Molinier, R. *et al.* Unsupervised topological learning approach of crystal nucleation. *Sci Rep* **12**, 3195 (2022). https://doi.org/10.1038/s41598-022-06963-5

Generative Modelling - Solidification

Task 1: Train on entire trajectory and generate random atomic configurations up to a cutoff distance.

Task 2: Train a conditional model that can optionally create solid (C1, C2) or liquid structures (C3, C4, C5, C6) on demand.

The validity of the structures will be checked by matching the radial and angular distributions as well as distribution of forces.

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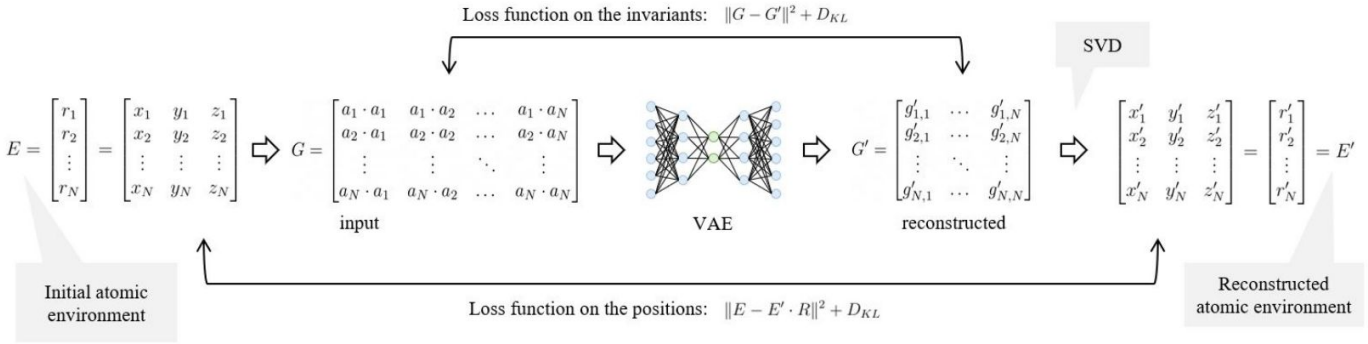
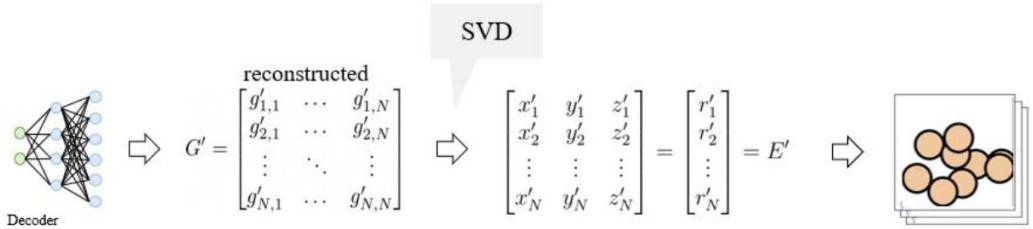
Generative Modelling - Solidification

Training



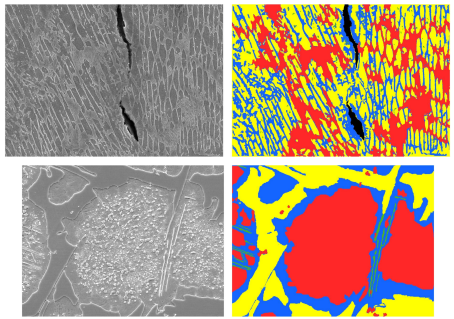
Generating

Draw n_Z samples from $\mathcal{N}(0, 1)$



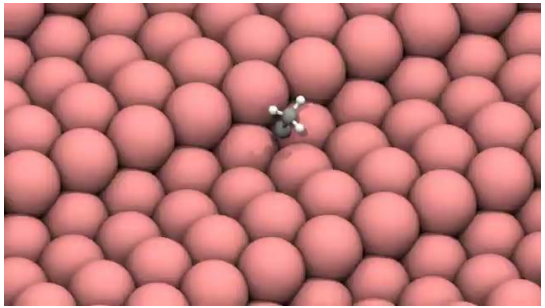
Challenges

Image Segmentation



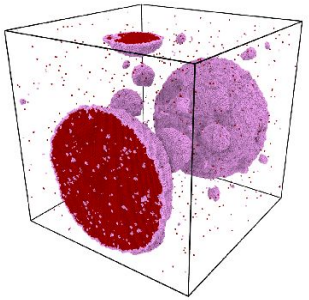
Skills involved:
Convolutional neural networks, image manipulation, regression, clustering

Interaction Potentials



Skills involved:
Atomic descriptors, (graph) neural networks, supervised learning

Generative Modelling



Skills involved:
Generative modelling, statistics, MD trajectory analysis, diffusion models, variational autoencoders

Organisation

- Zulip - Slack like tool to be used for communication
  https://dgc2025.zulipchat.com/join/ay53jgnbu4yqfonfwtktpggf/

- Kaggle - Used as central hub for the three challenges (get data, code, submission of results, running of jupyter notebooks, etc)

Organisation

Computational resources

- Kaggle - 30 hours/week GPU
- Google colab - Free CPU + ~4 hours / day

Timeline

- 17/10/25 - Kick off
  tIme to choose challenge and form teams
- 24/10/25 - Challenges posted on Kaggle

  Challenge in progress!

- 30/01/26 - End of challenge, submission closed
  evaluation phase
- 02/02/26 - Announcement of results