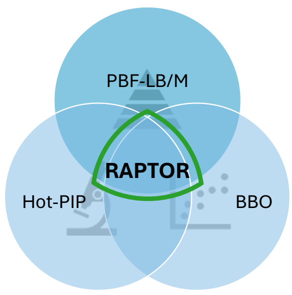
RAPTOR – Robust high-temperature mAterial discovery through ProbabilisTic Optimization foR additive manufacturing

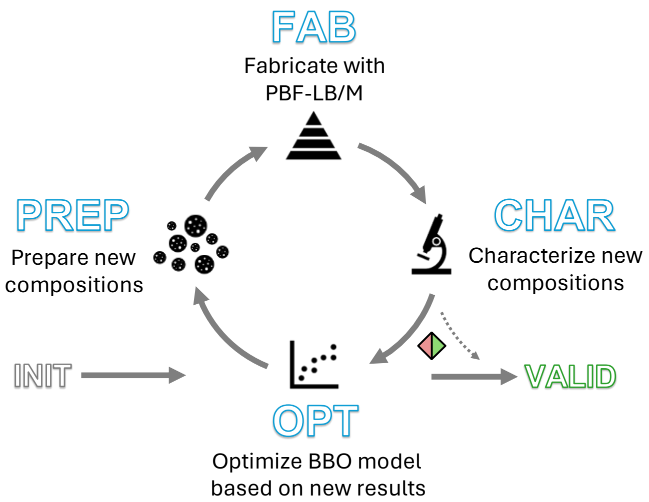


The project "RAPTOR – Robust high-temperature material discovery through probabilistic optimization for additive manufacturing" aims to improve material design by developing data-driven strategies for the discovery of new high-temperature materials. It focuses on optimizing materials for additive manufacturing (AM) using techniques such as black-box optimization (BBO) and high-temperature profilometry-based indentation plastometry (Hot-PIP). The project uses the laser-based powder bed fusion of metals AM method (PBF-LB/M, ASTM/ISO 52900) to create and find material compositions that perform better at high temperatures.

PBF-LB/M is effective for creating complex structures from difficult-to-machine materials, such as nickel-based superalloys, and enables the creation of new alloys by modifying powder mixtures. Traditional experimental design methods are costly and inefficient because they require numerous tests. RAPTOR aims to reduce unnecessary experiments by combining probabilistic modelling with iterative PBF-LB/M experiments. Data from these experiments will be used to train machine learning models using BBO methods such as Bayesian optimization (BO), which work well with limited data sets. The goal is to find the best powder blends for PBF-LB/M by balancing properties such as yield strength, elongation, hardness, and porosity.

Choosing the right machine learning model and training data is critical. To speed up testing and increase the number of possible experiments, RAPTOR uses Hot-PIP instead of standard tensile tests. Hot-PIP correlates well with traditional tensile testing and requires smaller specimens. The project also plans to collect additional data on properties such as porosity and hardness to improve the model's predictions. This data will be part of a black-box optimization loop to refine powder compositions and their material properties.

The goal of RAPTOR project is to find the Pareto front representing the optimal compositions of powder blends for the PBF-LB/M process. For example, the powder composition is the input (e.g., wt.% of base superalloy and additives), and the resulting properties) are the output (e.g., yield strength, elongation, hardness, and porosity). The Pareto front are the optimal powder blends that balance the different material properties.



The RAPTOR experiment loops include following steps:

- INIT - Initial experiment setup, determination of initial powder mixtures and results.
- PREP - Preparation of powder mixtures, mixing base powder with additive powders.
- FAB - PBF-LB/M fabrication and optional post-processing, sample fabrication.
- CHAR - Sample testing, including Hot-PIP, hardness and porosity measurements.
- OPT – Update of the BBO model with new data to refine its predictions for the next iteration. Check the stopping criterion, and return to PREP step or finish the loop if the criterion is met.
- VALID - Finally, the Pareto front is found – validate the results using alternative measurement techniques.

While RAPTOR focuses on nickel-based superalloys and PBF-LB/M additive manufacturing method, its results could benefit other areas of materials science and can find applications in various engineering scenarios.