BUTTERFLIES Project

Bio-Polymers & Additive Manufacturing

Newsletter II

The ML-Models in the Loop

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The ML-Models in the Loop

How BUTTERFLIES tries to automatically turn early experimental data into actionable "try this next" recommendations

In BUTTERFLIES, process development spans multiple manufacturing and formulation tracks. Across them, the bottleneck is the same: **finding the right parameter combinations efficiently is a multi-parameter optimisation problem**. Small changes in material composition, process settings, or environment can flip outcomes from robust parts to failed runs—and brute-force trial-and-error is slow and expensive.

VAL is building the **AI/ML optimisation layer and early prototypes** that connect structured data capture to predictive models and, ultimately, to **recommendations for the next best experiments**. The goal is to accelerate learning across the project while reducing wasted material, time, and energy.

From "trial-and-error" to a learning loop

Our approach is to create a practical optimisation loop that connects three pieces:

1. **Consistent data capture (DRA-aligned)**

   We rely on structured, comparable inputs: process variables (e.g., binder viscosity, droplet volume, saturation, curing profiles), material descriptors (powder/binder properties), and context (e.g., humidity/temperature, machine state).

2. **Predictive models that work with sparse, messy reality**

   Early in a project, data is limited and heterogeneous. That's why BUTTERFLIES focuses on methods that can learn effectively from small datasets while quantifying uncertainty. Crucially, this approach is designed to **improve continuously as the consortium generates more data**. Each new batch of validated results expands the covered parameter space, reduces uncertainty, and helps the models learn more reliable relationships—so recommendations become **more accurate, more robust, and more actionable** over time.

3. **Recommendations that researchers can act on**

Recommendations are meant to be directly actionable for process experts: not "a model in a notebook", but a ranked set of next experiments (and the expected trade-offs in accuracy, surface finish, throughput, and resource use).

Importantly, we are building this as a **modular** system. As new techniques emerge—and as we learn which model architectures perform best for BUTTERFLIES use cases—we can **swap components in and out** without rebuilding the full pipeline. In other words, the technology choices are **not set in stone**; the framework is designed to evolve with the project.

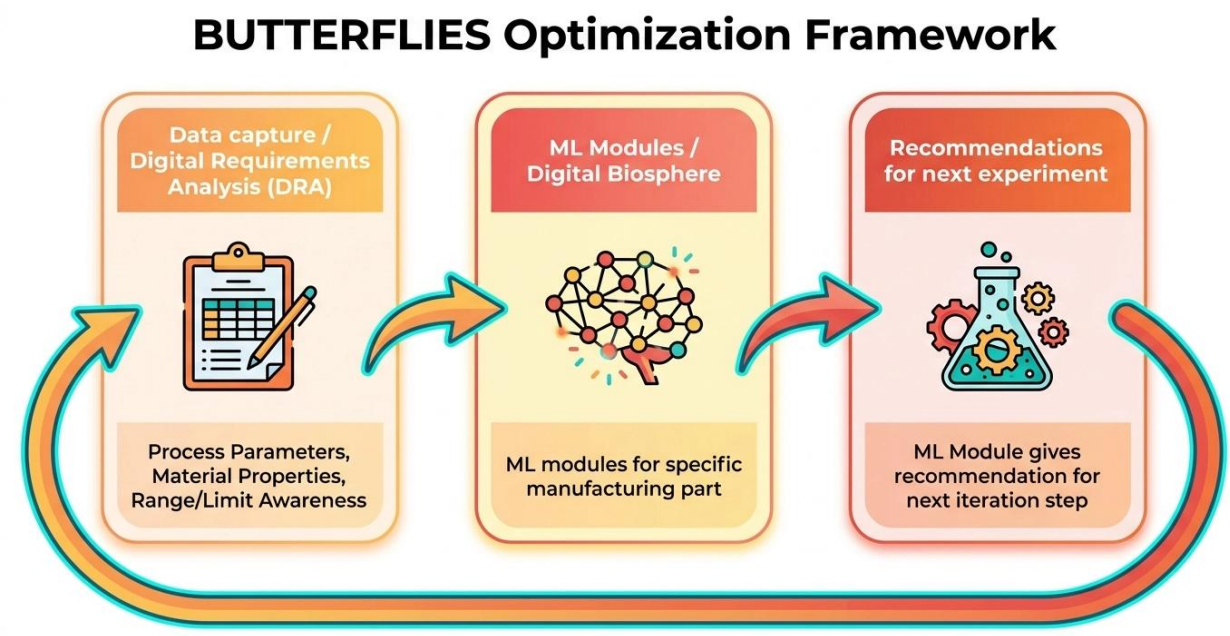

Figure 1: The BUTTERFLIES Optimization Framework guides experiments in a closed learning loop. From structured data capture to ML-driven recommendations aiming to **reduce the number of trials** needed to reach target performance, thereby **cutting material consumption, labor and overall costs**.