

Digital Medicines Manufacturing (DM²): AI-Driven Optimization of Oral Solid Dosage Form Development

MADE SMARTER
INNOVATION

DM²
Digital Medicines Manufacturing

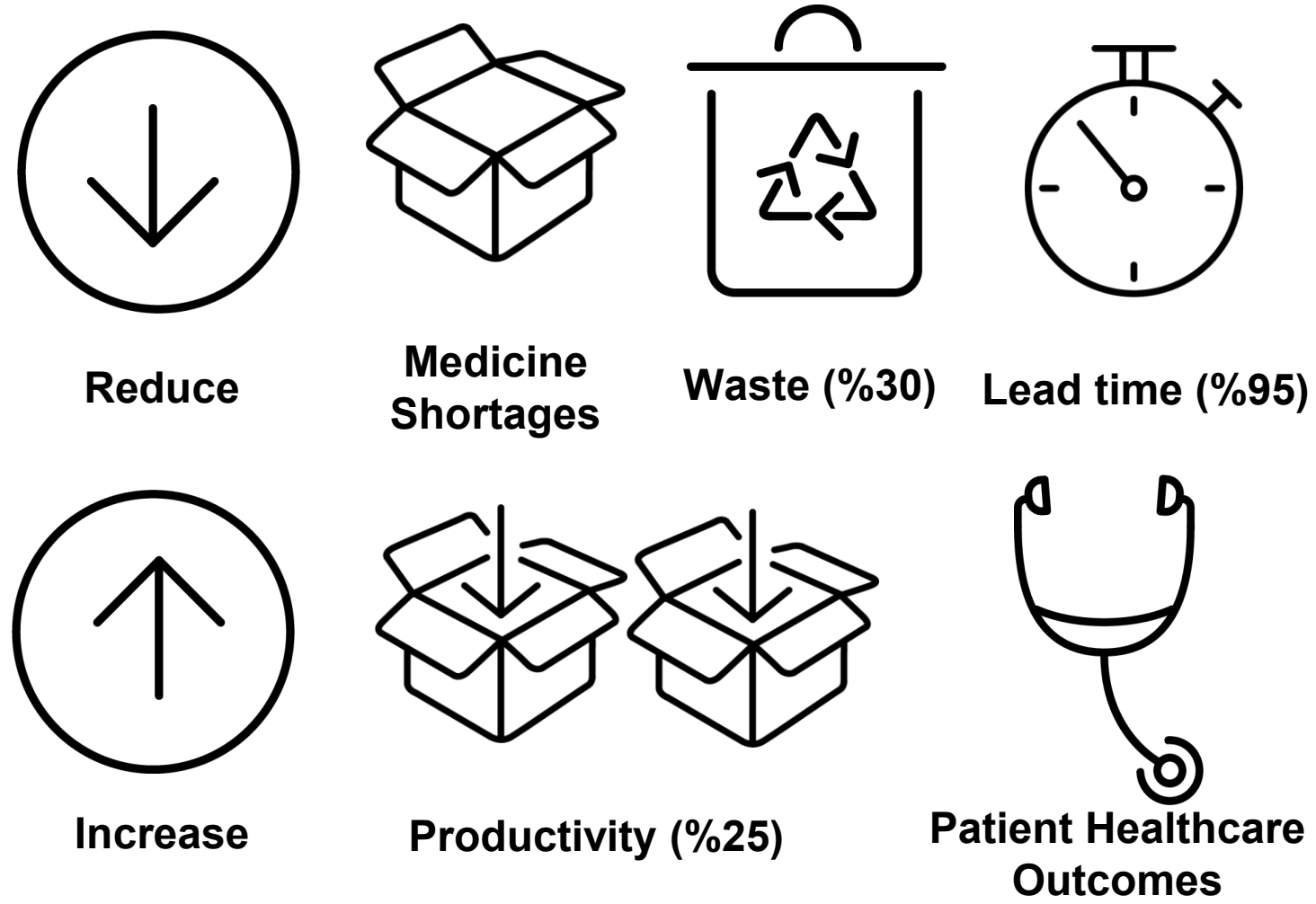
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Introduction to DM² Platform II

DM² Platform II uses AI technologies to develop an autonomous workflow for drug product manufacturing and testing system by identifying critical material attributes (CMAs) and associated critical process parameters (CPPs) that result in targeted critical quality attributes (CQAs). We aim to collect and use a database of 100s historical/new experiments to de-risk and accelerate drug product development while reducing experiments, development time, and materials use by 30%.



Overview of Manufacturing Optimization

The goal is to maximize the value of information from each experiment while minimizing the material consumption in order to 1) make the right material and 2) test the right property at the right time. The iterative, model-based optimization smartly designs the experiments, collects multi-scale and multi-point data, and updates the model to learn from the experiments.

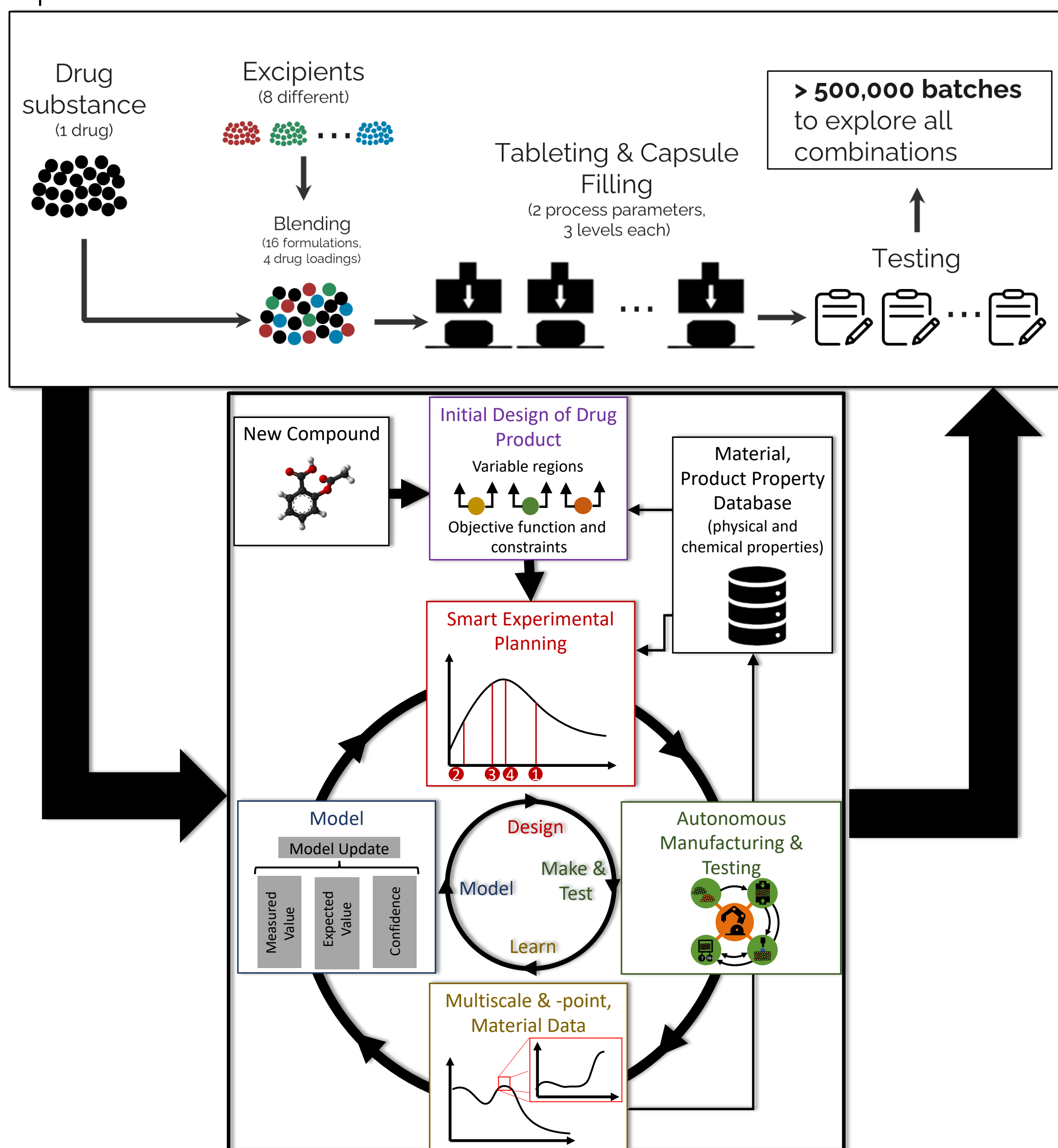


Figure 1: Challenges and the diagram of iterative drug product development process.

Problem Definition for Manufacturing Optimization

Different use cases were identified based on the specified input parameters, constraints, objectives and decision parameters. The framework is divided into two sub-problems, process and formulation optimization, where an outer loop (process optimization) is followed by an inner loop (formulation optimization). The goal is to enable flexible choice of different objectives/constraints at each level based on their relative importance.

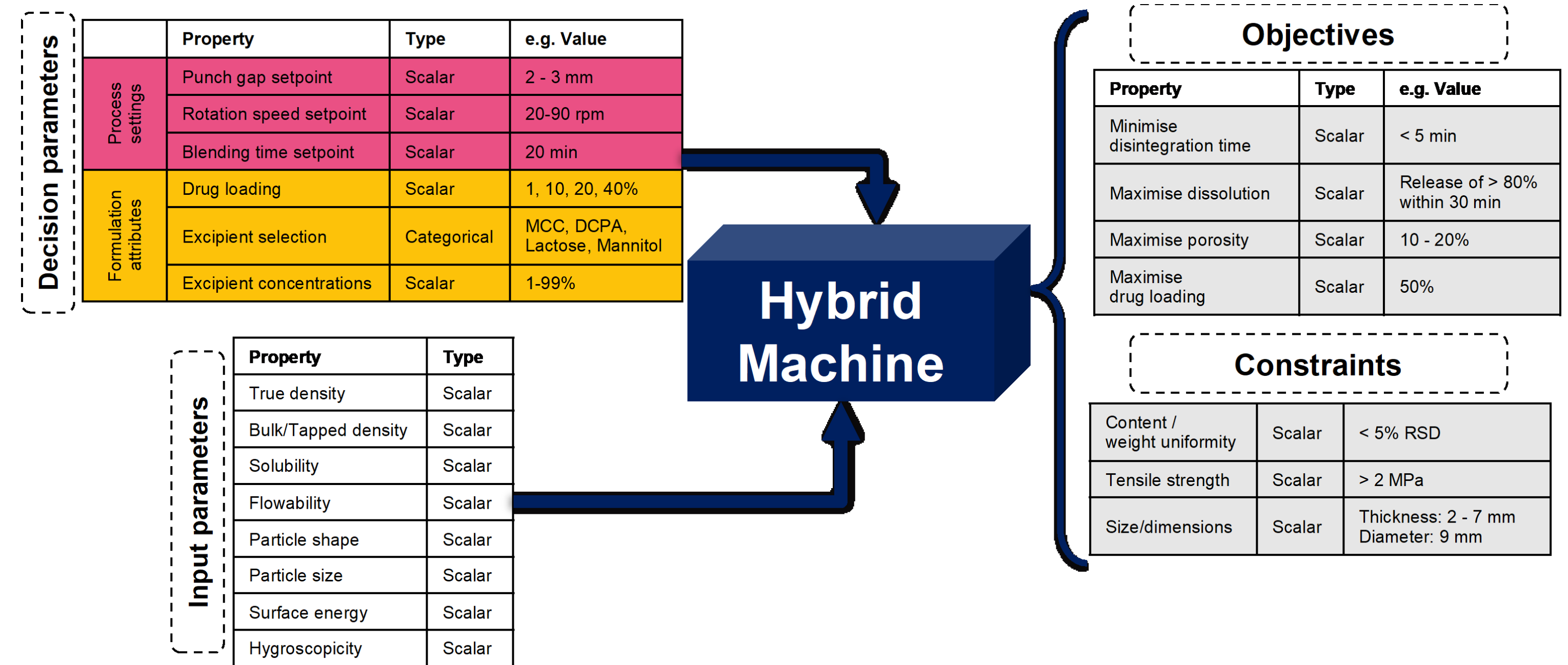


Figure 2: Schematic representation of the optimization workflow based on hybrid machine, including different decision and input parameters, objectives, constraints, and objectives.

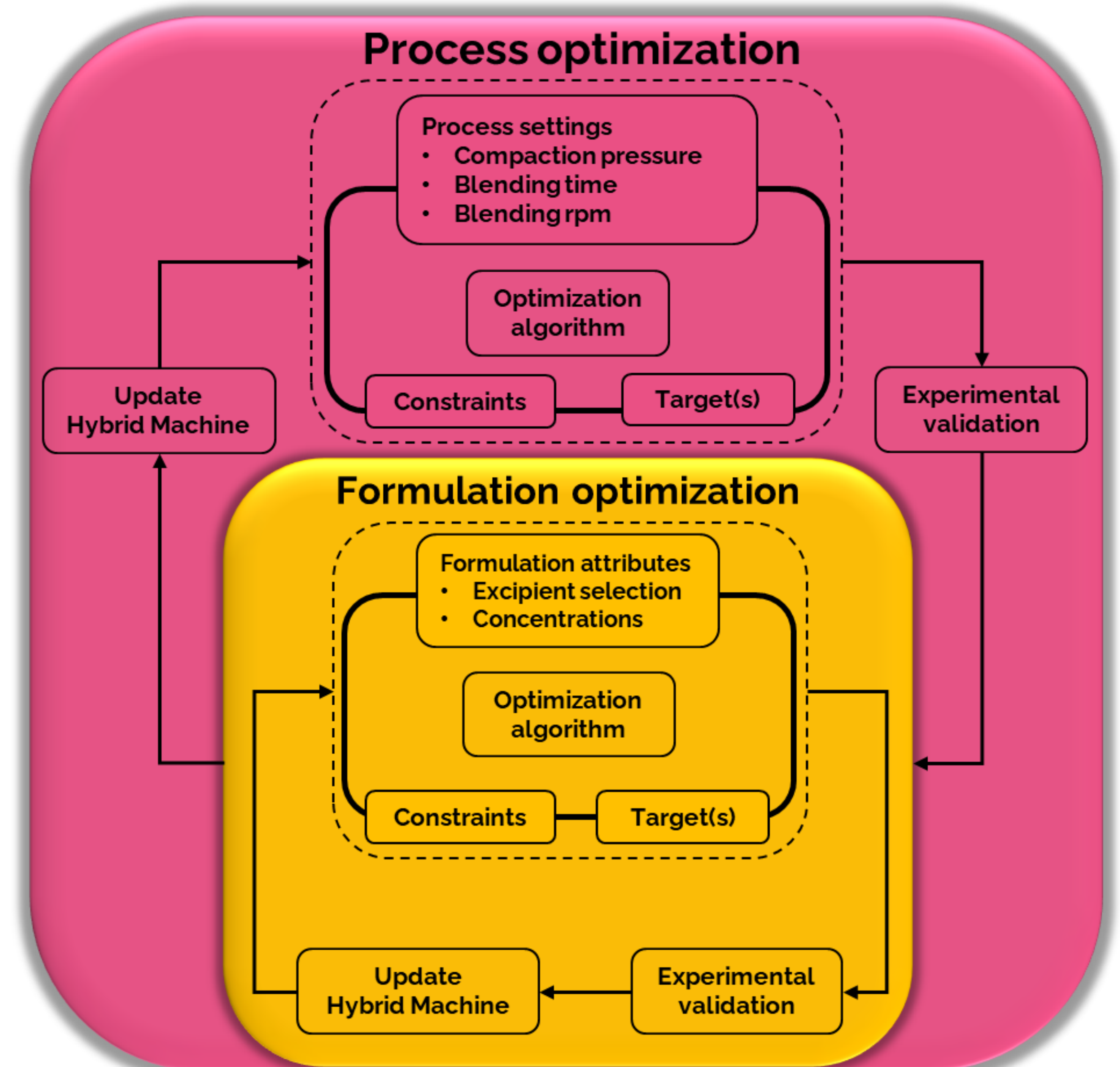


Figure 3: Flow diagram of the multi-level optimization framework for iterative, simultaneous optimization of process.

Modelling of Tablet & Capsule Attributes

To predict the product attributes, a hybrid machine is proposed to utilize historical data of raw material and blends imported into both domain knowledge (existing empirical/mechanistic models) and AI-based models (where domain knowledge is not available/reliable). The proposed approach is compatible with both tablet and capsule attribute prediction after implementing in the optimisation framework to optimize the targeted CQAs.

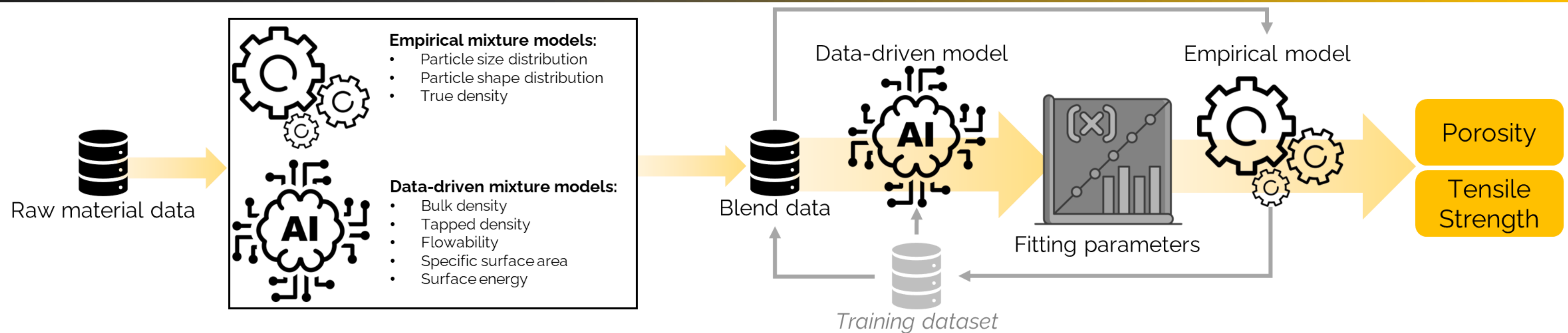


Figure 4: The proposed hybrid machine based on machine learning and empirical/mechanistic models to predict tablet/capsule attributes.

Three-Stage Roadmap for Model-based Drug Development Optimization

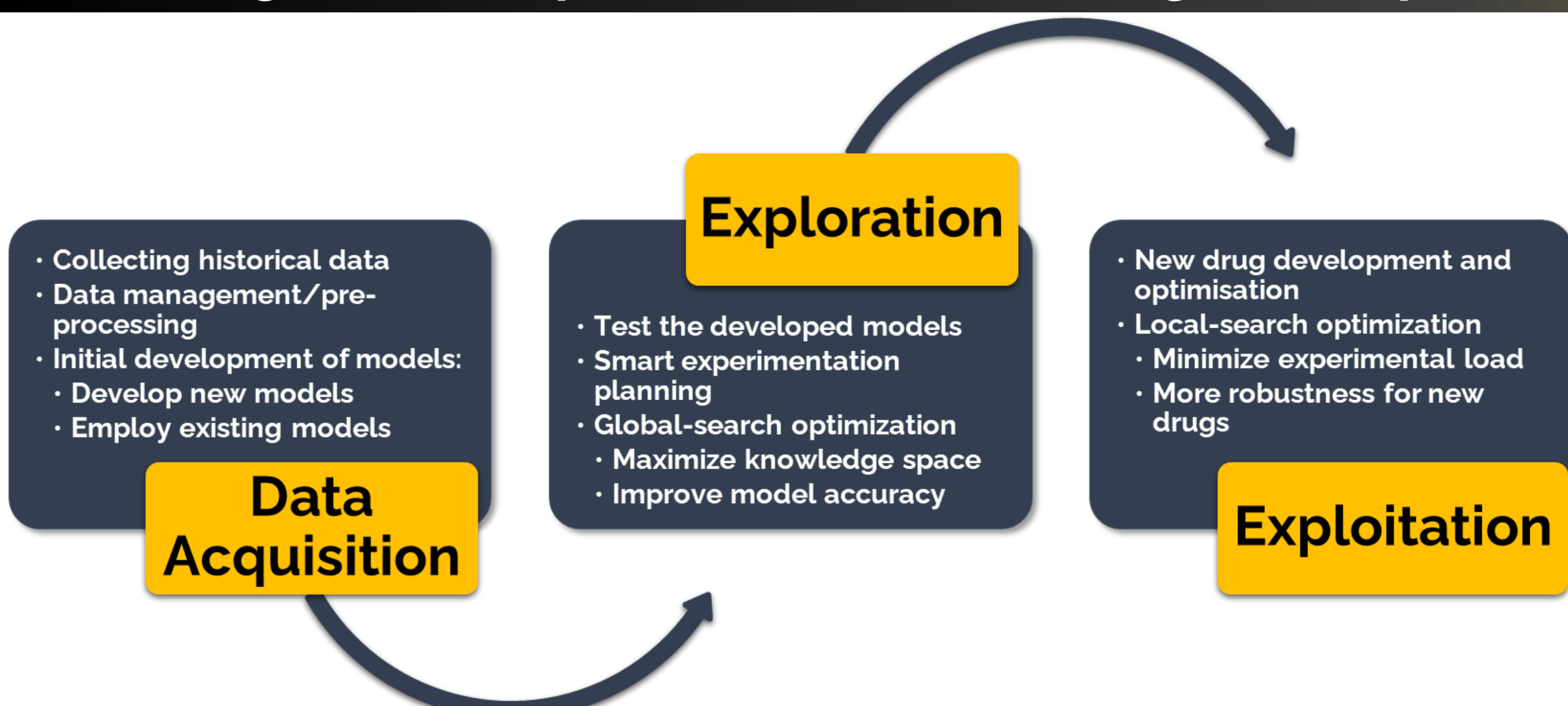


Figure 5: The three-stage roadmap towards development of an autonomous microscale drug manufacturing system.

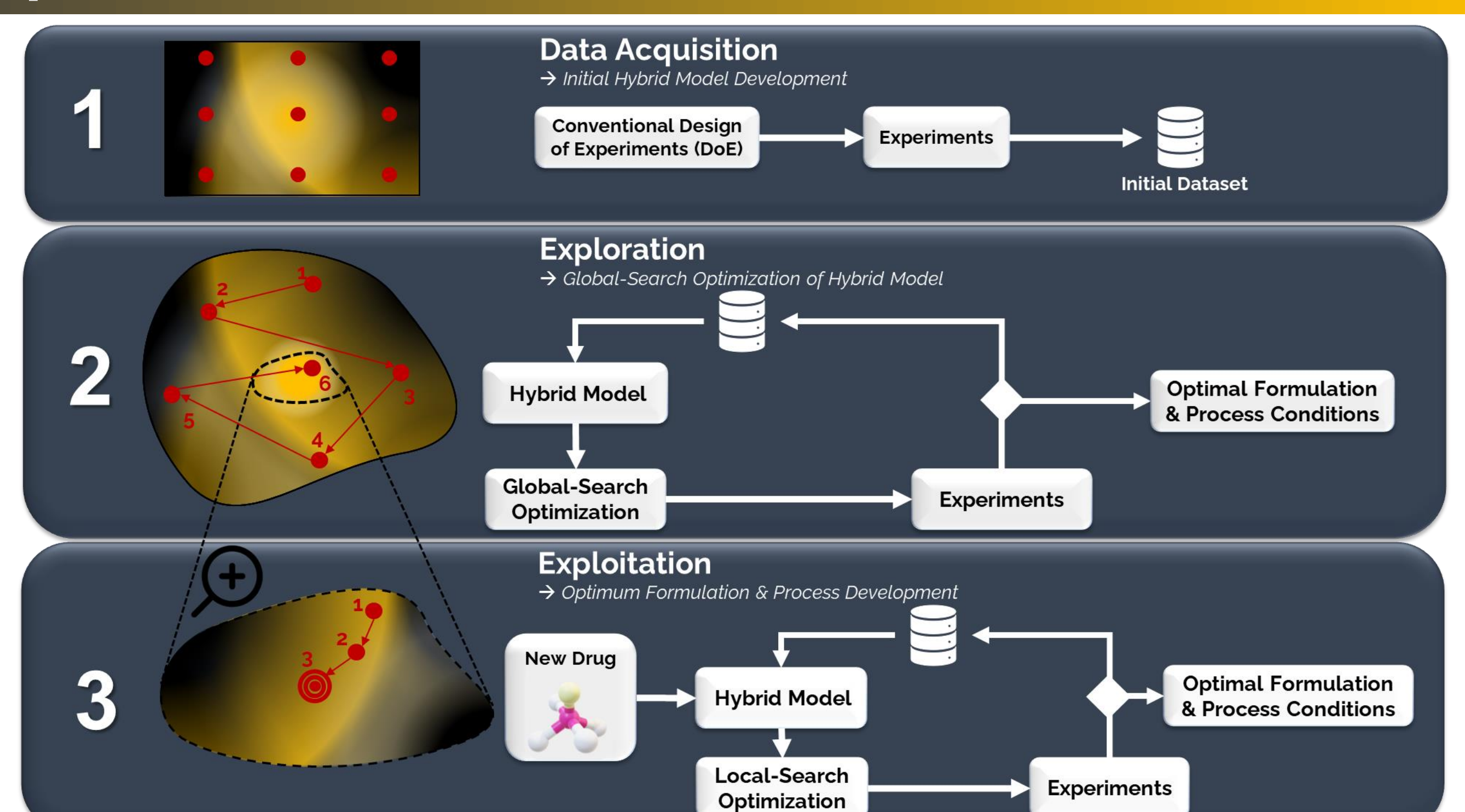


Figure 6: Adaptive use of global-search and local-search optimization algorithm in different stages of modelling and optimisation of new drug development.



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