confidential

AI4b.io - Uniting AI and Bioscience

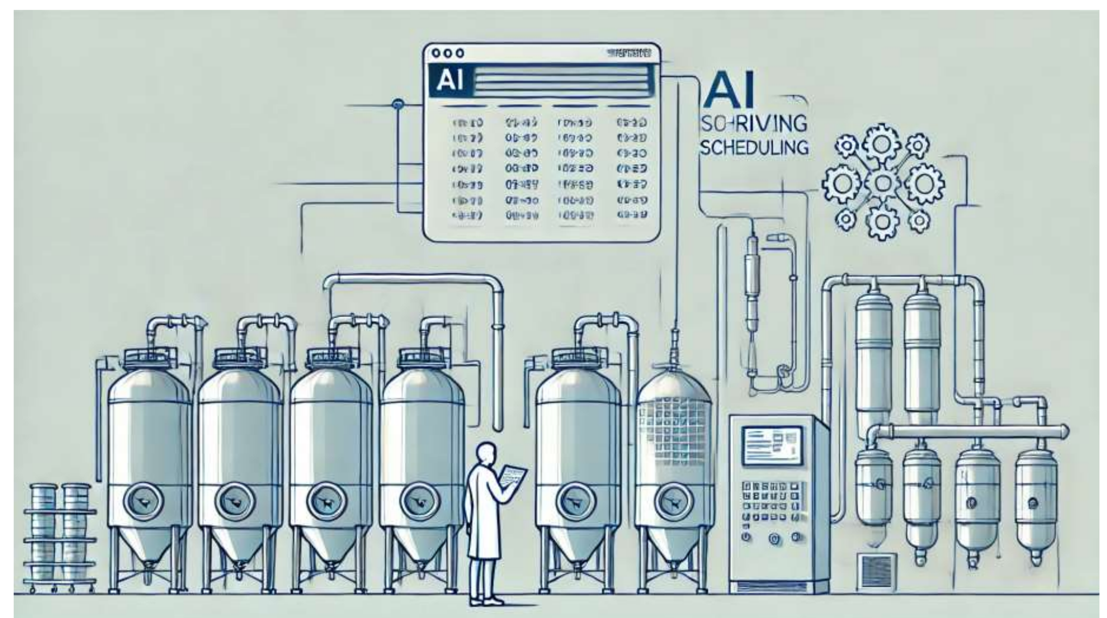
Kim van den Houten, Mahdi Naderibeni, Joery de Vries, Paul van Lent, Chengyao Peng, Esteban Freydell, David Tax, Mathijs de Weerdt, Liang Wu, Matthijs Spaan, Stijn Bierman, Joep Schmitz, Thomas Abeel, Ali May, Henk Noorman, Wouter van Winden, Hans Roubos, Renger Jellema, Jana Weber, Marcel Reinders

TU Delft Delft University of Technology
dsm-firmenich
ICAI Innovation Center for Artificial Intelligence

- **AI4b.io** advances AI in biosciences to drive sustainable innovation.
- The lab develops AI-driven methods for biobased products and production technologies, enhancing research and industrial efficiency.
- Fully funded by dsm-firmenich and the RVO.

Digital Twin and Smart Plant Scheduling: By integrating AI models into plant scheduling, this project enables smart allocation of resources in biomanufacturing, improving efficiency in both scheduling and production. It reduces downtime and enhances flexibility across the production pipeline.

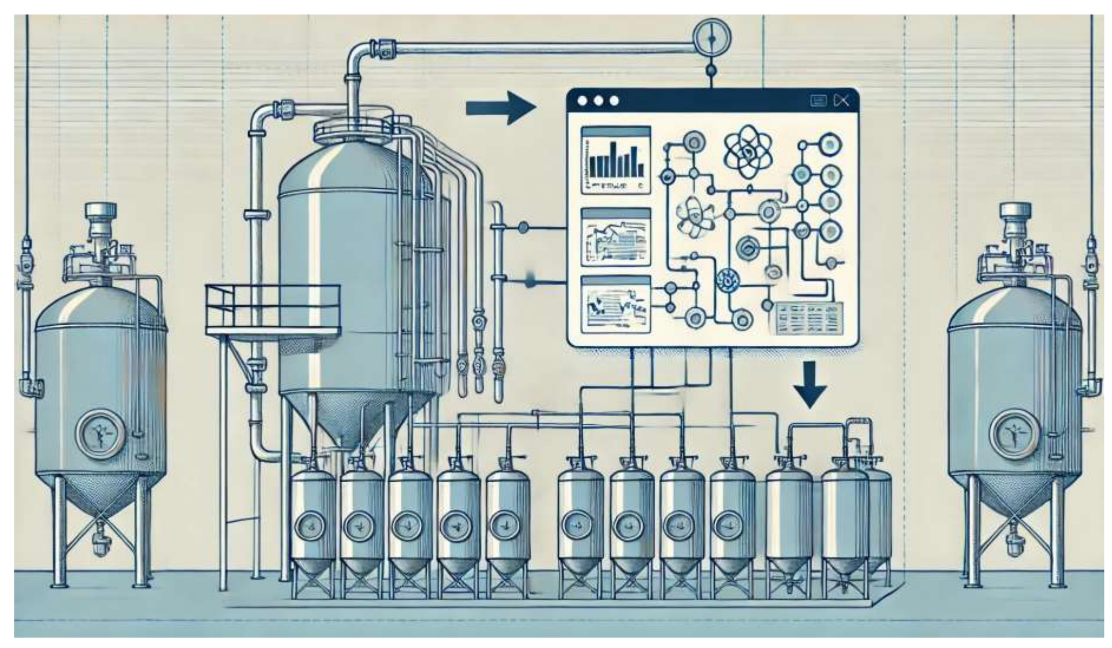
Kim van den Houten Kim van den Houten explores scheduling algorithms for biomanufacturing under uncertainty. Her work addresses the challenge of creating schedules that are both optimal and robust by investigating if deterministic representations can simplify stochastic models. Leveraging decision-focused learning, she uses score function gradient estimation to develop practical, solvable scheduling models [1].



[1] *Learning From Scenarios in the Context of Stochastic Repairable Scheduling.* K. van den Houten, D.M.J. Tax, E. Freydell, M. de Weerdt, CPAIOR 2024.

AI-Assisted Fermentation Digital Twin: This project creates a digital twin that simulates and monitors fermentation in real time, enabling researchers to optimize bio-production by predicting outcomes, adjusting variables, and reducing trial-and-error in scaling bio-manufacturing processes.

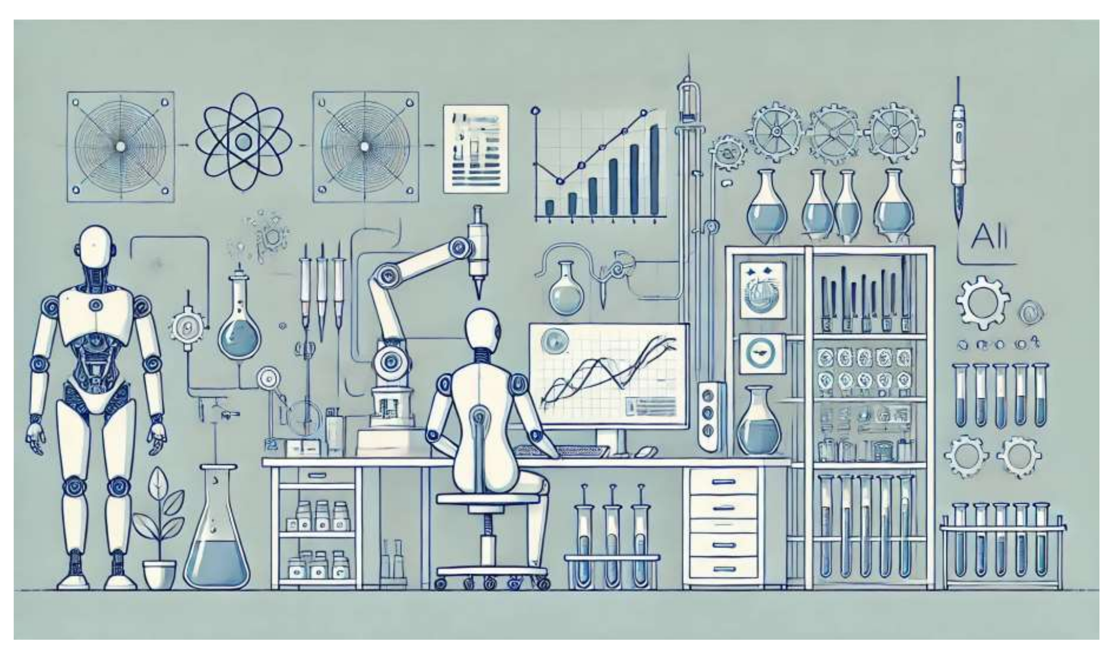
Mahdi Naderibeni integrates machine learning, fluid dynamics, and bio-process modeling for faster prediction, monitoring, and optimization of industrial fermentation. Using CFD simulations and in situ measurements, he employs physics-informed machine learning to enhance process efficiency, addressing the complexities of bio-production through advanced modeling techniques [2].



[2] *Learning solutions of parametric Navier-Stokes with physics-informed neural networks.* M. Naderibeni, M. J. Reinders., L. Wu, D. M. Tax, arXiv:2402.03153 2024.

AI for Self-Driving Laboratories: This project develops fully automated laboratories where AI algorithms autonomously run and optimize experiments. The self-organizing labs boost experimental throughput, reproducibility, and accelerate bioscience innovation by minimizing manual intervention.

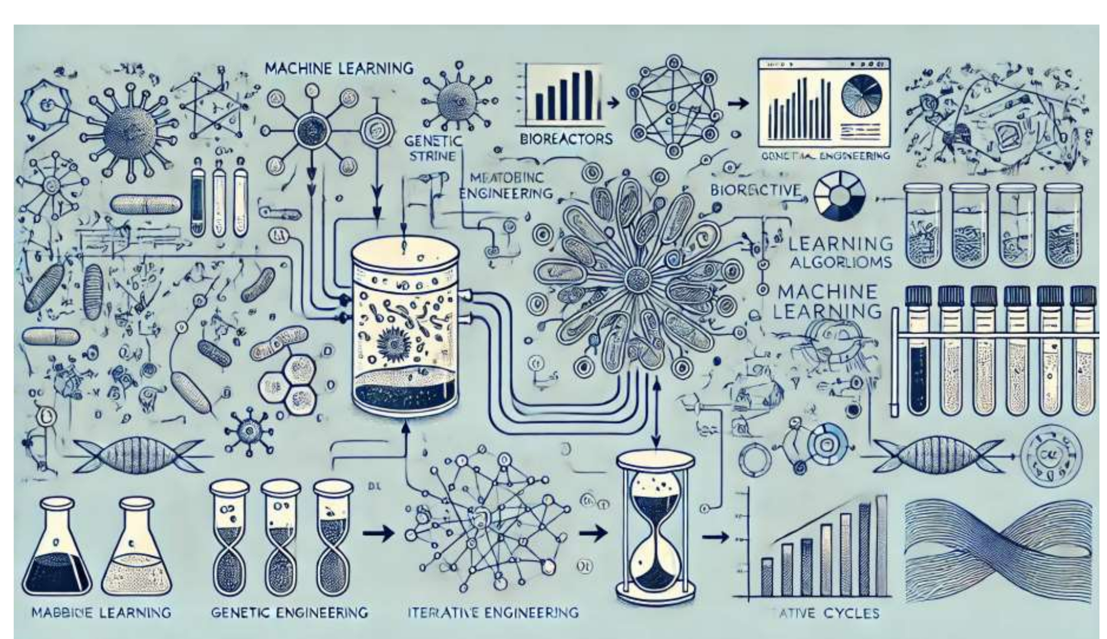
Joery de Vries explores optimal experiment design in self-driving labs, balancing exploration and exploitation. He uses Bayesian optimization under simplified lab assumptions and reinforcement learning for broader, adaptable strategies. A key study examines uncertainty management in black-box agents, enhancing model robustness, exploration, and predictive intervention [3].



[3] *Bayesian Meta-Reinforcement Learning with Laplace Variational Recurrent Networks.* Joery de Vries, Jinke He, Mathijs de Weerdt, Matthijs Spaan. EWRL 2024.

Machine Learning for Iterative Metabolic Engineering: Focused on enhancing microbial strain design, this project uses machine learning to iteratively improve genetic engineering. It accelerates development cycles, optimizing microbial processes that produce bio-materials for food, health, and industry.

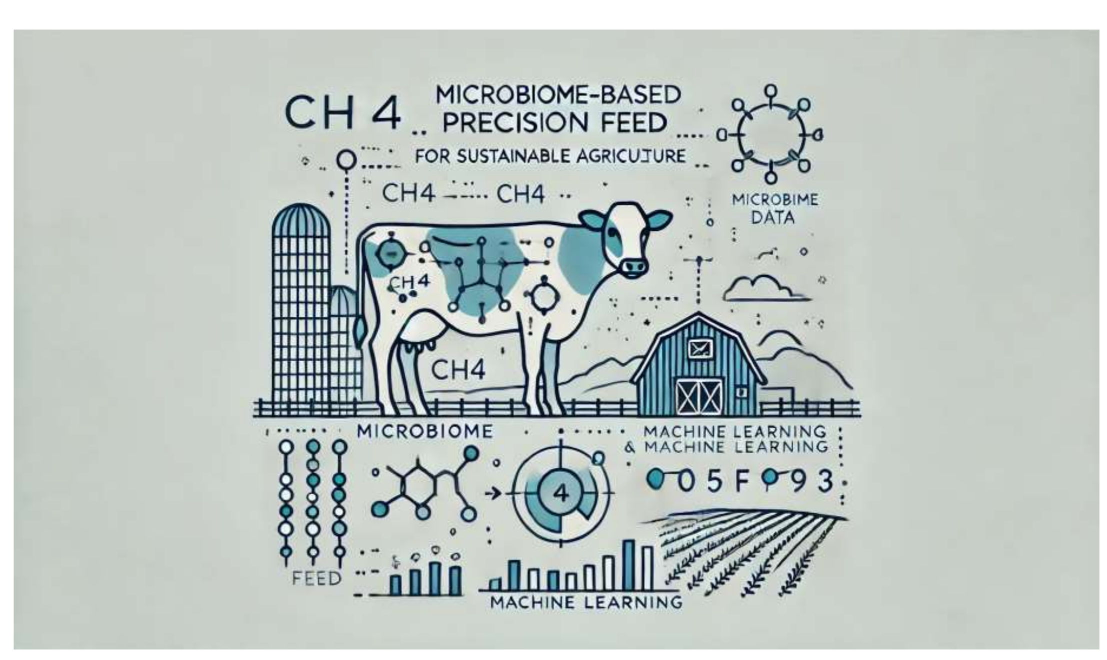
Paul van Lent applies and develops supervised ML methods integrated with automated recommendations for the Design-Build-Test-Learn (DBTL) cycle. He uses a kinetic model-based simulation tool to compare ML algorithms for metabolic engineering. This simulation-guided approach optimizes DBTL parameters, enhancing microbial strain design [4].



[4] *Simulated design–build–test–learn cycles for consistent comparison of machine learning methods in metabolic engineering.* P. van Lent, J. Schmitz, T. Abeel. ACS Synthetic Biology 2023.

Microbiome-Based Precision Feed: This project applies machine learning to tailor animal feed based on microbiome data, supporting precision nutrition. By optimizing feed for specific microbiome profiles, it aims to improve animal health and promote sustainable agriculture.

Chengyao Peng applies machine learning to address the complexity of microbiota-based solutions in animal phenotypes. Using big data and holo-multi-omics, supervised ML predicts cow methane emissions and identifies key rumen microorganisms, informing future feed development. Statistical and self-supervised methods enhance precision nutrition strategies.



[5] *Unveiling microbial biomarkers of ruminant methane emission through machine learning.* C. Peng, A. May, T. Abeel. Frontiers in Microbiology, 14: 1308363, 2023.

Interested to learn more or collaborate? Please contact us through info@ai4b.io