MicrobesGym: development of a virtual arena to explore deep learning algorithms applied to bioprocess microbiomes

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What is microbesGym?

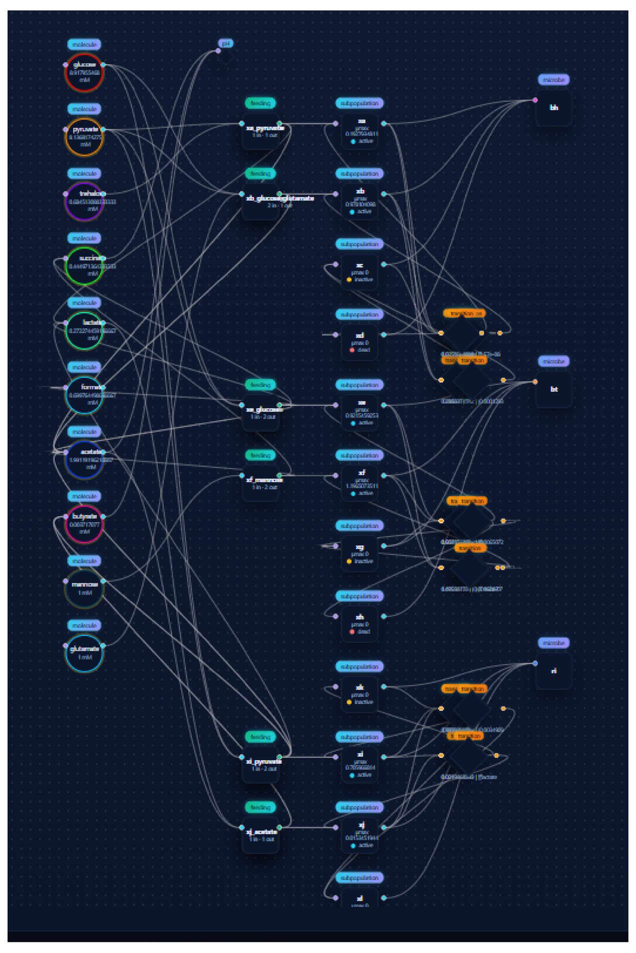
A virtual arena to build **kinetic microbiome models**, simulate them, and optimize their environments using **deep reinforcement learning**.

microbeGym consists of two components:

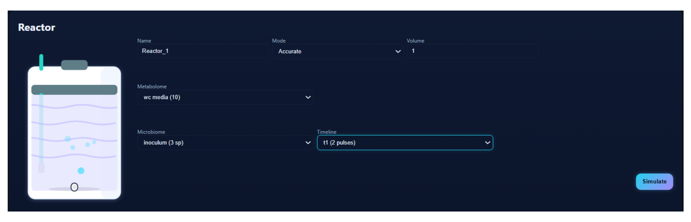
1) **Simulation engine** to build customized kinetic models of microbial process.

2) A **Gymnasium-like environment** to train deep-reinforcement agents to optimize specific microbiome functions.

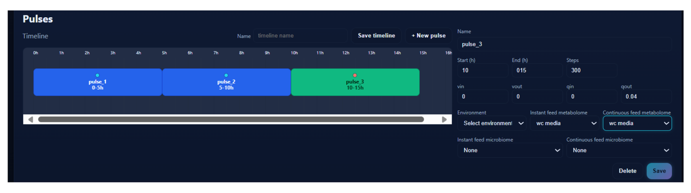
Simulation Engine



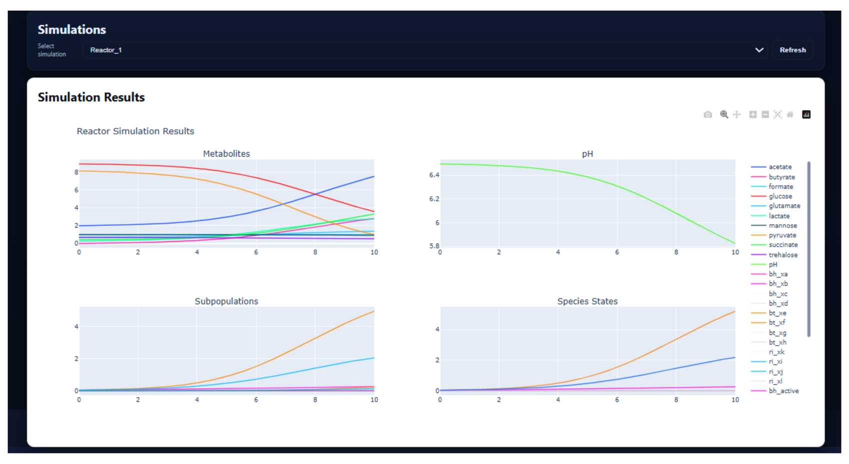
1. Build your kinetic model.



2. Build your virtual reactor.

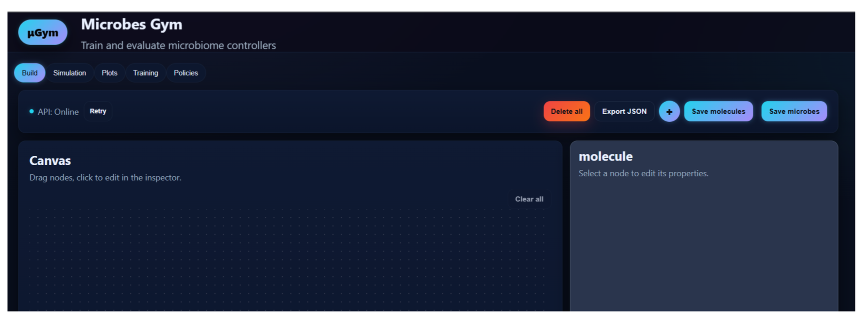


3. Define control pulses (pH, stirring, feeding, inoculation, etc.)

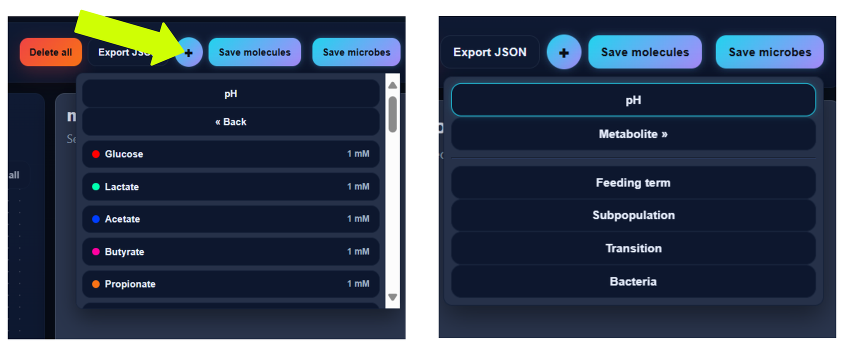


4. Simulate.

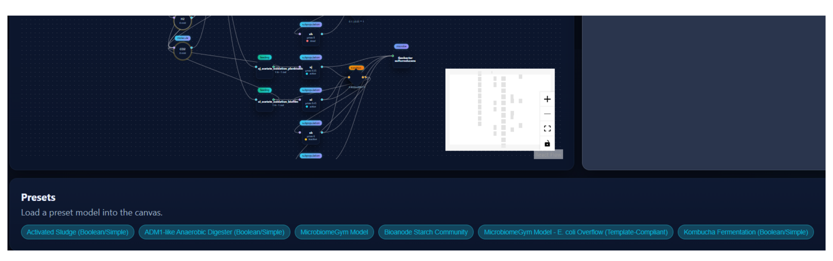
1. Intuitive User Interface



Main canvas.

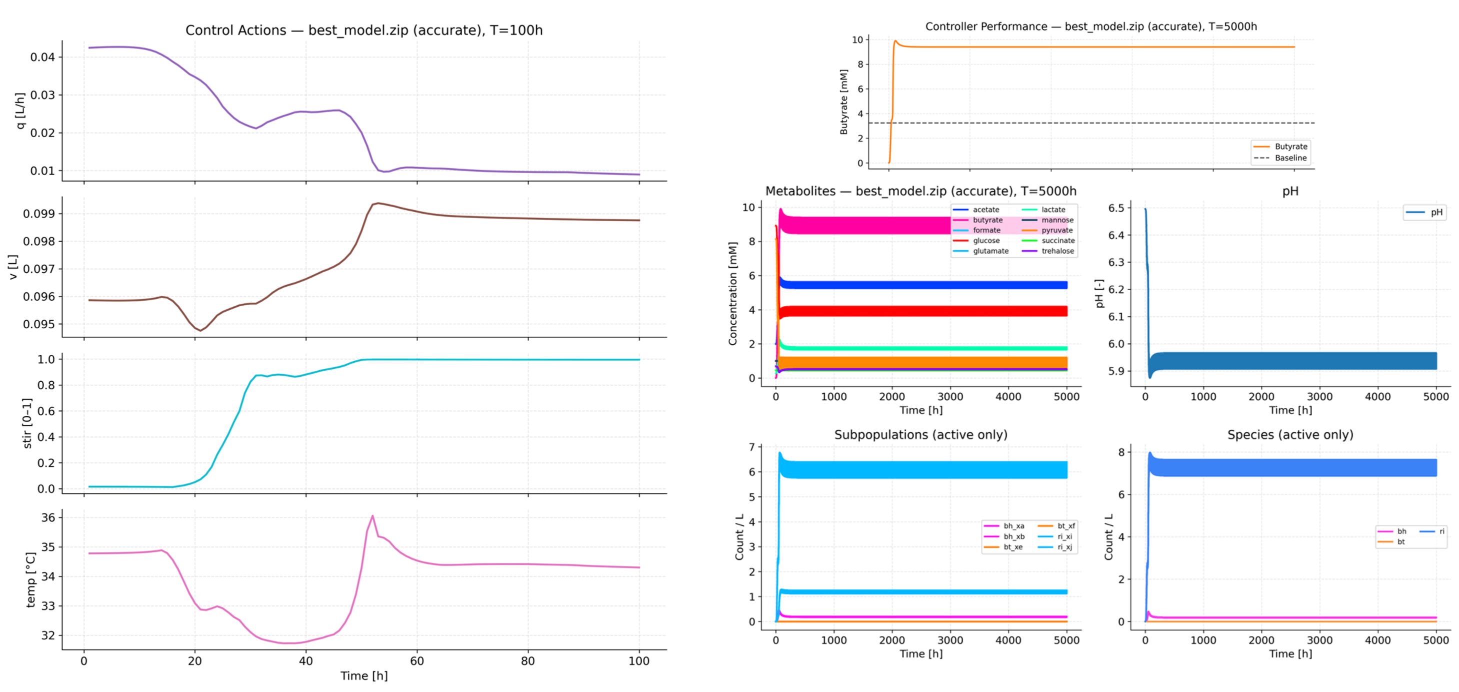


Add molecules, microbes, and kinetic terms.



Use a preset model. *E.g.*, activated sludge, bioanode, synthetic gut community, and kombucha fermentation

Gymnasium Environment



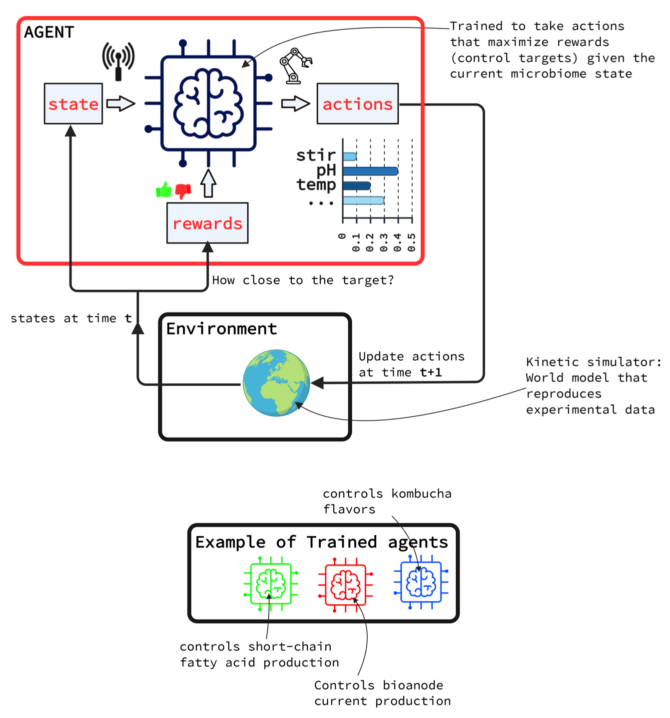
1) Define the actions that the agent can take (stir, temperature, pH, dilution rates, feeding molecules, etc.;
2) Define a goal based on one or more components of the systems;
3) Select the algorithm (SAC, PPO, TD3, etc);
4) Train the agent;
5) Use it to control your system.
Example of an agent trained to maximize butyrate production in a synthetic gut microbial community.

Deep reinforcement learning

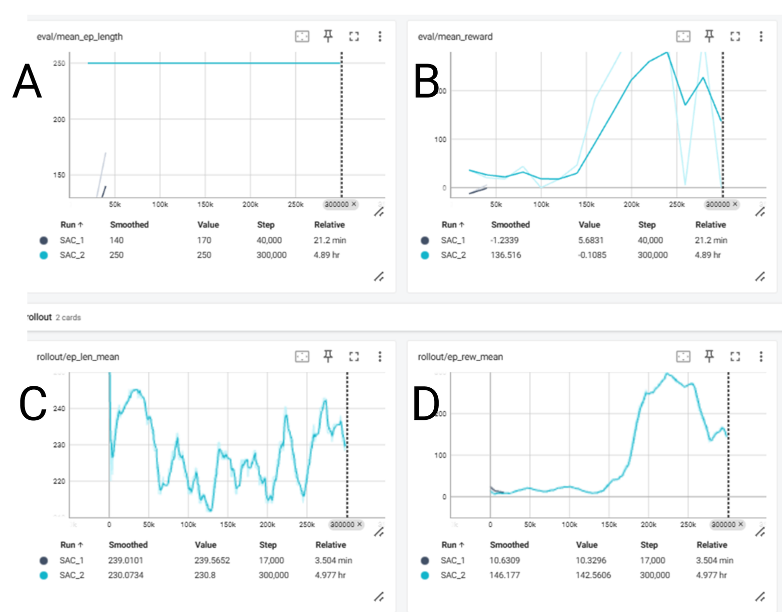
Definitions

Deep Reinforcement leaning trains agents to learn optimal actions by interacting with an environment and maximizing rewards. It combines deep neural networks with trial-and-error exploration, enabling adaptive feedback control without pre-programmed strategies.

Gymnasium environments are standardized, open source APIs for simulation reinforcement learning tasks. Facilitates rapid prototyping and comparison of algorithms.



MicrobesGym workflow. The **agent** is a decision making entity: observes the environment's state, chooses actions and updates its policies based on received rewards.



Agent in training. (A) and (B) evaluation rounds with fixed episode length of 250 hours. (C) and (D) training rounds.