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MS-BioNET Overview

MS-BioNET is a simulation framework for modelling and simulating large networks of compartments hosting a chemical solution and communicating through an enhanced model of chemical reaction addressing molecule transfer.

On top of the framework, a logic-oriented specification language is used to flexibly specify simulation scenarios: on the one side it tightly focusses on biochemistry, by providing constructs to directly express biochemical reactions, compartments, compartment link topology, and reactions involving selective transfer through membranes; on the other side it relies on logic-based goal resolution and unification, achieving the expressiveness needed to easily handle size and complexity of the biochemical network.

Behind the hood, such a specification is turned into an intermediate language (a sort of bytecode) that feeds a simulation engine implemented by adapting the optimised version of Gillespie's algorithm (Gibson and Bruck's paper) to the computational model of biochemical cell networks.