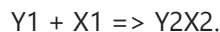
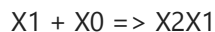


Cell Constructor

The goal of this project is to build an application that implements simulations of complex molecular behaviours using simple computational rules via an intuitive user interface.

Processes in living cells can seem magical at first sight - DNA is replicated faithfully at each cell division, independent signals are passed to the right recipients without crosstalk, the cell separates into two functional daughters, etc. Many of these behaviours can be described globally, ignoring the actual reactions that take place (e.g. cell divides), or locally via the reactions, without giving information about how this relates to the complex behaviour (e.g. $n\text{MP} + \text{ATP} \rightarrow n\text{MP-AMP} + \text{P}_2\text{O}_7$). The goal of this project is to help develop better intuition about these behaviours by defining them via local abstract rules, like $A + B \rightarrow C$, and simulate the outcome to obtain the global picture. More technically, you would implement a particle simulator that evolves according to a stochastic context free grammar that defines the transitions. The user interface would include both an area for determining the local rules, as well as a canvas for the global simulation.

As an example, consider a problem of DNA replication, where an exact copy of a long molecule is made. The process is relatively well understood, and could be written down as a large set of complicated differential equations. In a simplified abstract model, one could represent a single free-floating DNA base by X_0 (where X could be A,C,G,T), the base in a polymer by X_1 , and a paired one by X_2 . The greatly simplified replication process in a complicated molecular soup of A_0, T_0, C_0, T_0 , etc, could then be condensed to two rules:



There is a wide range of complex behaviours that can be reached with such simple relations. Similarly, there are many complicated biochemical models of cell behaviour that could be attempted to reduce to a small number of rules. Your work would allow people to define and explore them.

This educational product is aimed for scientists or educators who want to develop intuition about workings of biomolecules, and more generally, for people who like exploring how complex natural phenomena can be captured by computational rules. There is an existing basic simulator called OrganicBuilder (GPL v3 license) that achieves some of the goals set above. However, it lacks a nice interface, such as touch-aided controls, as well as more lifelike behaviours, such as different molecule sizes and diffusion rates, and stochastic execution of the rules. We have permission of the developer to fork and expand on this code base, if it is more reasonable than starting from scratch.

<https://github.com/BertrandDechoux/OrganicBuilder>

<https://bertranddechoux.github.io/OrganicBuilder>