Overview

We have constructed a tool for modeling the molecular interactions between HIV and a human T cell. From application of this tool, we gain a stronger understanding of HIV infection, with the ability to make inferences and discover trends from the simulation data that is generated. We plan to eventually release the codebase to the public once the user API is more developed, so that anyone can use and contribute to the codebase as well as run simulations to make their own inferences.

Currently, the available model features are as follows:

Run a particular simulation (supported user API)

Each simulation attempts to model a particular interaction between HIV and a human T cell. They each hold some state, and this state evolves as time passes in the simulation and some processes take place within the host cell environment (e.g., alternative splicing, degradation, mRNA export, Tat feedback). The initial state and how it changes over time may vary drastically from simulation to simulation, as factors like the site of HIV integration in the host genome heavily influences the characteristics of the interaction.

Generate simulation data in the form of plots and tables (supported user API)

Each simulation holds some state that changes over time as the host cell experiences changes from the processes that take place within the cell. This data is outputted at every timestep and can be plotted as a function of time (e.g., Rev protein count as a function of time). The data can also be exported in CSV format for independent processing and analysis. We can also plot data across multiple simulations and compute various statistics, like the average or standard deviation of the viral progeny production rate as a function of time. From these plots, we can make inferences or discover trends from the data. The model tool can also generate histograms for the simulation data at a particular timestep (for this final part, the user API is still being developed).

Parameter sensitivity analysis (supported user API)

Generally, the values of the physical parameters we employ in our model are drawn from the literature. We occasionally fit parameter values so that the simulation data output matches that of the literature when we can't find the parameter values directly. The user API provided by the model allows users to perform sensitivity analysis by having users choose a physical parameter and then changing its value slightly across simulations to see how the host cell environment changes in response.

Save and load individual model interactions (working but user API needs some development)

Since each simulation contains state information about the host cell conditions, we offer a feature to save this state and load it later on for further analyses. The user can either load the state to study information about a particular HIV-T cell interaction or continue the simulation (corresponding to the state) from where it was last stopped using this loaded state data.

Extensive test suite (working but user API needs some development)

As the state evolves over time in any particular HIV-T cell interaction, our test suite has the ability to check that the behavior indicated by the state is consistent with the literature and how we expect the model to behave. Tests that fail enable us to make the necessary model corrections, or sometimes may yield insight into how the interaction behaves differently from what we initially expected, giving us a better understanding of the model.