

Agent Based Modeling and Simulation of Biomolecular Reactions

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We present a dynamic, agent-based, three-dimensional model of the phage lambda gene regulatory system. The phage lambda is a virus which infects the host bacteria *Escherichia coli* and reproduces itself passively in the lysogenic phase. However, UV radiation triggers lytic growth resulting in a spurt of virus reproduction.

We use the agent-based approach to model the processes that constitute the switching from lysogenic to lytic states and vice-versa. In an agent based model, the constituents of a complex system are modeled as agents and the overall behavior of the system is a result of interaction among these agents. The system is built with a bottom-up approach, using the agents and so the system is more accurately modeled. This approach has the benefit of allowing us to isolate and study the effect of various individual parameters on the overall behavior of the system. This approach is thus an alternative to the traditional top-down approach based on differential equations and stochastic simulation.

The model is being developed using *breve*, an Integrated Development Environment (IDE) developed by Jon Klein. *breve* has its own language, *steve* and a 3-D visualization engine and can run on both Windows and Linux. The components of the gene regulatory system are modeled as multiple decentralized agents. Agents have properties and a set of local interaction rules among themselves, and evolve to exhibit complex behaviors leading to the desired switching mechanism of the lambda circuit. The whole emergent behavioral patterns can be simulated and displayed using the 3-D engine. Our work extends that done by Glorious Tsui at University of Calgary, Canada and provides open-source versions of the system components.

To design our system and to allow other researchers to model their systems in a similar way, we developed the Unified Modeling Language (UML) model of the system with well-defined objects, methods and use cases. The UML constructs can be used as modifiable templates for system components and interactions. Thus our approach can be applied to study a wide range of biomolecular reactions.

This work was motivated originally by a project to model sensors and digital computing gates built from biochemical components. But our approach is also applicable to any system of biomolecular reactions including those of interest in areas such as physiology, pharmacology and medicine. These computational components have many applications in areas such as healthcare, environmental monitoring and homeland security.