

An Agent-Based Approach to Modeling Membrane Formation

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Cell membranes play a crucial role in the lives of cells. Because they are selectively permeable to ions and organic molecules, membranes are central to regulating the state of a cell. How does the structure of a cell membrane arise and why is it so prevalent in nature across many life forms? The cell membrane arises through a process of self-assembly. Indeed, molecular self-assembly is ubiquitous throughout biological systems. This project presents a simplified model of molecular self-assembly of cell membranes that shows the simple computational mechanism that enables self-assembly to work. Understanding the sufficient conditions under which self-assembly can occur helps us identify instances of self-assembly as well as further enabling us to take advantage of it for the synthesis of biological components. We present an agent-based model that demonstrates self-assembly of a variety of higher-level structures through the use of simple mechanics. Using simulation strategies such as dissipative particle dynamics, past models have focused on matching natural phenomena at a quantitative level. Our model dispenses with many details of the physical processes involved, employing a simpler set of rules, yet still demonstrates the qualitative properties seen in self-assembly, explaining the puzzle of its ubiquity in nature. The model is an agent-based model that contains three agent types: water, hydrophobes, and hydrophiles. The agents follow simple rules in which they move towards or away from random neighbors depending on their types.

Models such as the one presented here exemplify a computational thinking approach to science, and can have powerful roles in education. They allow scientists and learners to engage with complex phenomena such as self-assembly in an intuitive yet rigorous fashion. Research has demonstrated the difficulties students have in understanding emergent processes such as self-assembly. Agent-based models have been shown to help students make sense of emergent phenomena. We designed a lesson plan for high school biology students based around this model. This model has been used in high school classrooms to help students gain a better understanding of how membrane formation works. In our presentation, we will describe the details of the model, demonstrate it, and report on the results of the school implementations.