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Agent-Based Modeling Investigating Self-Organization in Open, Non-equilibrium Thermodynamic Systems

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Abstract : This research applies the power of agent-based modeling to a pivotal question at the intersection of biology, computer science, physics, and complex systems theory about the self-organization processes in open, complex, non-equilibrium thermodynamic systems. Central to this investigation is the principle of Maximum Entropy Production (MEP). This principle suggests that such systems evolve toward states that optimize entropy production, leading to the formation of structured environments. It is hypothesized that guided by the least action principle, open thermodynamic systems identify and follow the shortest paths to transmit energy and matter, resulting in maximal entropy production, internal structure formation, and a decrease in internal entropy. Concurrently, it is predicted that there will be an increase in system information as more information is required to describe the developing structure. To test this, an agent-based model is developed simulating an ant colony's formation of a path between a food source and its nest. Utilizing the Netlogo software for modeling and Python for data analysis and visualization, self-organization is quantified by calculating the decrease in system entropy based on the potential states and distribution of the ants within the simulated environment. External entropy production is also evaluated for information increase and efficiency improvements in the system's action. Simulations demonstrated that the system begins at maximal entropy, which decreases as the ants form paths over time. A range of system behaviors contingent upon the number of ants are observed. Notably, no path formation occurred with fewer than five ants, whereas clear paths were established by 200 ants, and saturation of path formation and entropy state was reached at populations exceeding 1000 ants. This analytical approach identified the inflection point marking the transition from disorder to order and computed the slope at this point. Combined with extrapolation to the final path entropy, these parameters yield important insights into the eventual entropy state of the system and the timeframe for its establishment, enabling the estimation of the self-organization rate. This study provides a novel perspective on the exploration of self-organization in thermodynamic systems, establishing a correlation between internal entropy decrease rate and external entropy production rate. Moreover, it presents a flexible framework for assessing the impact of external factors like changes in world size, path obstacles, and friction. Overall, this research offers a robust, replicable model for studying self-organization processes in any open thermodynamic system. As such, it provides a foundation for further in-depth exploration of the complex behaviors of these systems and contributes to the development of more efficient self-organizing systems across various scientific fields.

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