Biological pattern-forming systems characterized better through geometry than simulations

November 23 2020

Like the collective motions of bird flocks, the patterns result from the concerted interactions of many individual particles without a central coordinator. Credit: CC0 Public Domain

Ludwig-Maximilians-Universitaet (LMU) in Munich physicists have introduced a new method that allows biological pattern-forming systems

to be systematically characterized with the aid of mathematical analysis. The trick lies in the use of geometry to characterize the dynamics.

Many vital processes that take place in biological cells depend on the formation of self-organizing molecular patterns. For example, defined spatial distributions of specific proteins regulate cell division, cell migration and cell growth. These patterns result from the concerted interactions of many individual macromolecules. Like the collective motions of bird flocks, these processes do not need a central coordinator. Hitherto, mathematical modeling of protein pattern formation in cells has been carried out largely by means of elaborate computer-based simulations. Now, LMU physicists led by Professor Erwin Frey report the development of a new method which provides for the systematic mathematical analysis of pattern formation processes, and uncovers the their underlying physical principles. The new approach is described and validated in a paper that appears in the journal *Physical Review X*.

The study focuses on what are called 'mass-conserving' systems, in which the interactions affect the states of the particles involved, but do not alter the total number of particles present in the system. This condition is fulfilled in systems in which proteins can switch between different conformational states that allow them to bind to a cell membrane or to form different multicomponent complexes, for example. Owing to the complexity of the nonlinear dynamics in these systems, pattern formation has so far been studied with the aid of time-consuming numerical simulations. "Now we can understand the salient features of pattern formation independently of simulations using simple calculations and geometrical constructions," explains Fridtjof Brauns, lead author of the new paper. "The theory that we present in this report essentially provides a bridge between the mathematical models and the collective behavior of the system's components."

The key insight that led to the theory was the recognition that alterations

in the local number density of particles will also shift the positions of local chemical equilibria. These shifts in turn generate concentration gradients that drive the diffusive motions of the particles. The authors capture this dynamic interplay with the aid of geometrical structures that characterize the global dynamics in a multidimensional 'phase space." The collective properties of systems can be directly derived from the topological relationships between these geometric constructs, because these objects have concrete physical meanings—as representations of the trajectories of shifting chemical equilibria, for instance.

"This is the reason why our geometrical description allows us to understand why the patterns we observe in cells arise. In other words, they reveal the physical mechanisms that determine the interplay between the molecular species involved," says Frey. "Furthermore, the fundamental elements of our theory can be generalized to deal with a wide range of systems, which in turn paves the way to a comprehensive theoretical framework for self-organizing systems."

More information: Fridtjof Brauns et al, Phase-Space Geometry of Mass-Conserving Reaction-Diffusion Dynamics, *Physical Review X* (2020). DOI: 10.1103/PhysRevX.10.041036

Provided by Ludwig Maximilian University of Munich